

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032123\
 Data File : VX034652.D
 Acq On : 21 Mar 2023 14:16
 Operator : JC/MD
 Sample : 02013-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 215

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\82X031023W.M
 Title : SW846 8260

Signal : TIC: VX034652.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.050	153	158	172	rBV	352370	567600	4.32%	1.260%
2	2.373	205	211	216	rBV	130422	216837	1.65%	0.482%
3	2.532	229	237	249	rBV	94717	182323	1.39%	0.405%
4	4.556	559	569	588	rBV	75064	218939	1.67%	0.486%
5	5.001	630	642	657	rBV3	88747	301400	2.29%	0.669%
6	5.385	694	705	721	rBV2	144135	421577	3.21%	0.936%
7	5.550	721	732	748	rVB	256220	727430	5.53%	1.615%
8	5.952	785	798	812	rBV	175274	467970	3.56%	1.039%
9	6.763	921	931	945	rBV	398910	972535	7.40%	2.160%
10	8.647	1234	1240	1247	rBV	836181	1317339	10.02%	2.925%
11	8.720	1247	1252	1259	rVB	313773	485180	3.69%	1.077%
12	10.055	1465	1471	1482	rVB	855479	1157179	8.80%	2.570%
13	11.079	1634	1639	1647	rBV	708357	896506	6.82%	1.991%
14	12.018	1788	1793	1801	rVB	857021	1124441	8.55%	2.497%
15	12.103	1801	1807	1818	rVB	710363	963920	7.33%	2.141%
16	12.219	1821	1826	1840	rBV	1451113	2133078	16.22%	4.737%
17	12.792	1917	1920	1927	rVB2	218578	349784	2.66%	0.777%
18	12.859	1927	1931	1946	rBV	2890960	4257233	32.38%	9.454%
19	12.975	1946	1950	1957	rBV	596520	1170728	8.90%	2.600%
20	13.073	1961	1966	1968	rVV	814314	1261093	9.59%	2.801%
21	13.103	1968	1971	1973	rVV2	4339990	5779066	43.95%	12.834%
22	13.128	1973	1975	1988	rVV	7170135	13148774	100.00%	29.200%
23	13.225	1988	1991	2008	rVB	1172184	3147533	23.94%	6.990%
24	13.426	2020	2024	2034	rBV	471586	883523	6.72%	1.962%
25	13.512	2034	2038	2046	rVV	426398	672729	5.12%	1.494%
26	13.591	2047	2051	2061	rVB4	226143	455018	3.46%	1.010%
27	13.756	2072	2078	2080	rBV4	85231	169895	1.29%	0.377%
28	13.896	2094	2101	2113	rBV3	147751	518227	3.94%	1.151%
29	14.579	2208	2213	2220	rBV	230369	552504	4.20%	1.227%
30	14.688	2229	2231	2243	rVB2	117483	243104	1.85%	0.540%
31	14.792	2243	2248	2251	rBV3	143315	266720	2.03%	0.592%

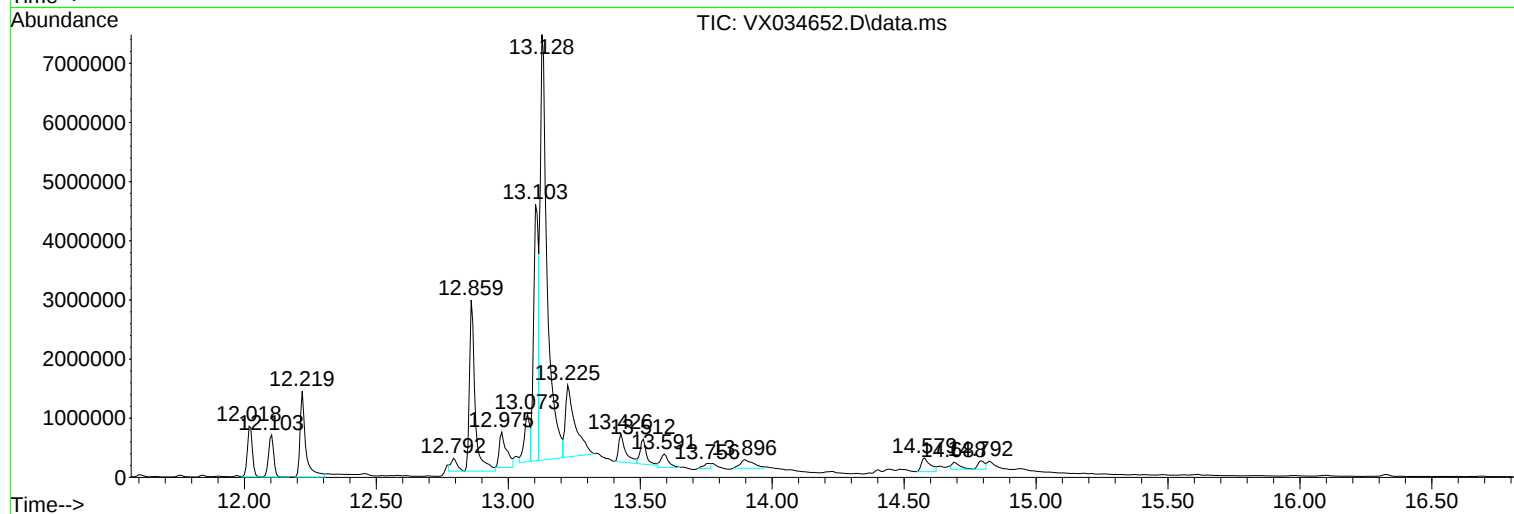
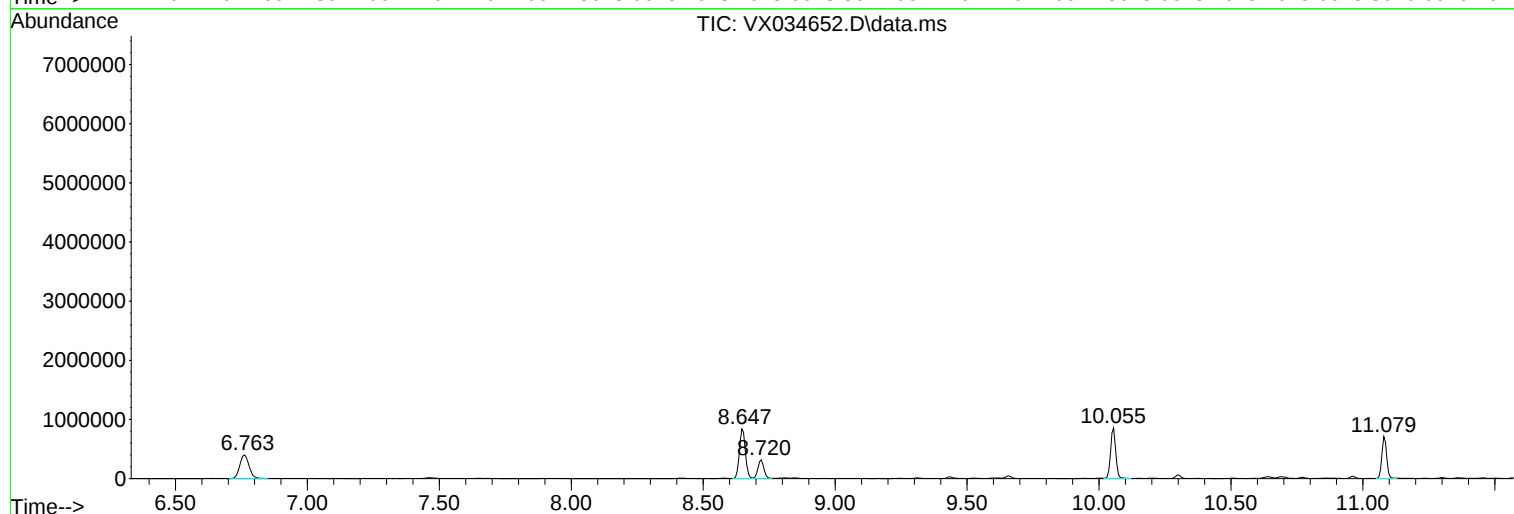
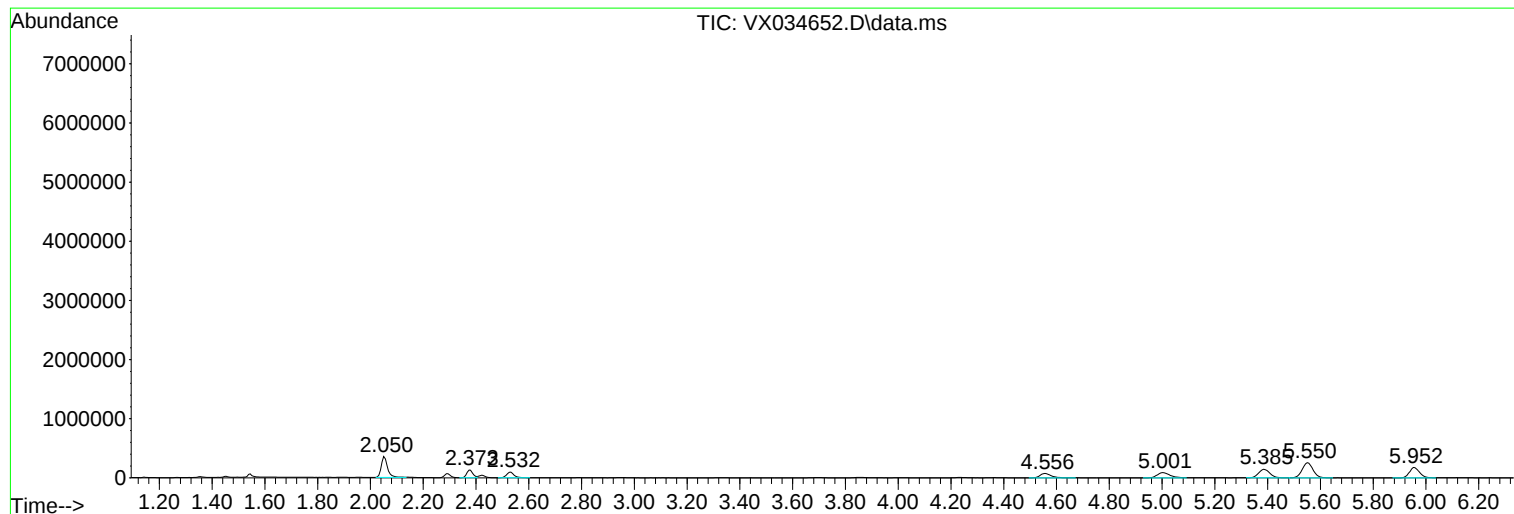
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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



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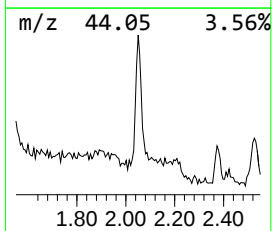
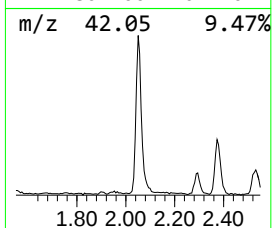
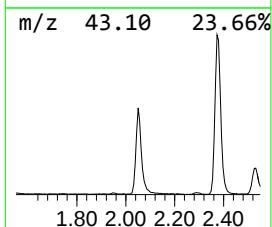
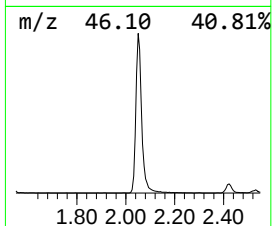
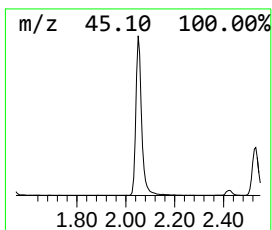
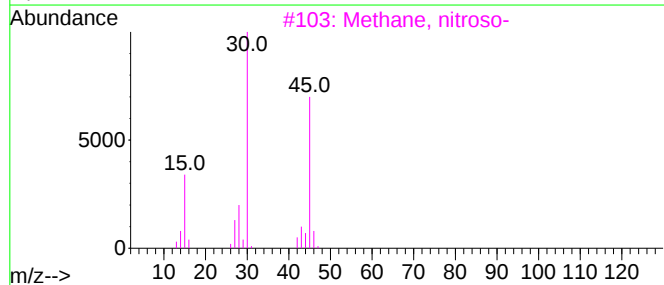
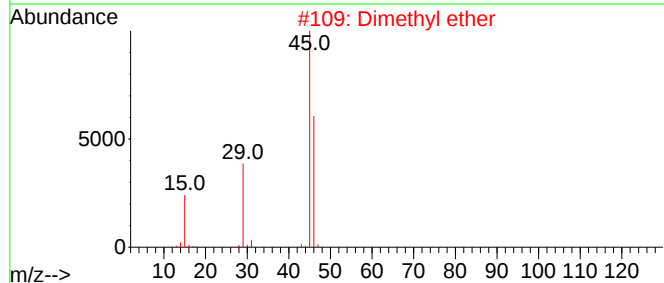
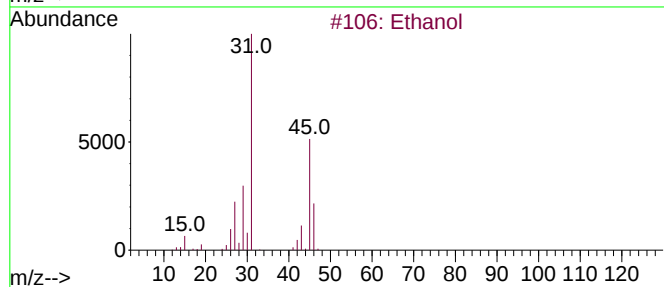
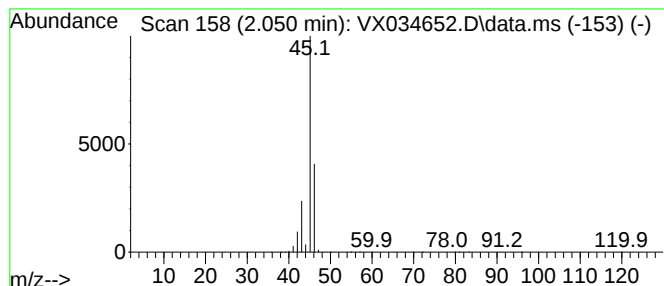
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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.
2.050	39.01 ug/l	567600	Pentafluorobenzene	5.550

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol		46	C2H6O	000064-17-5	64
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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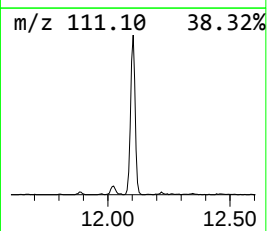
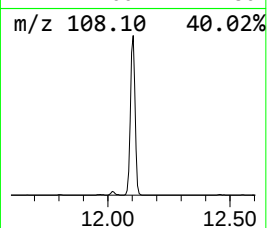
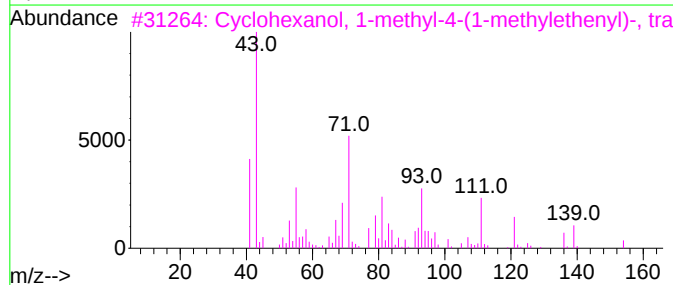
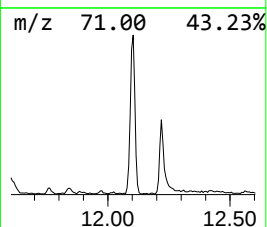
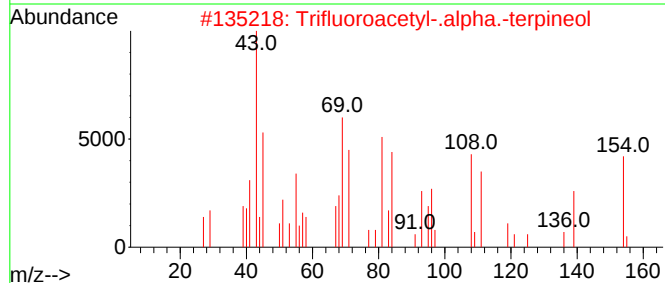
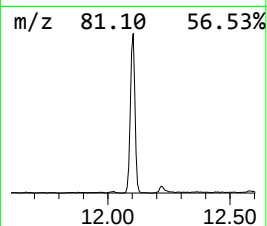
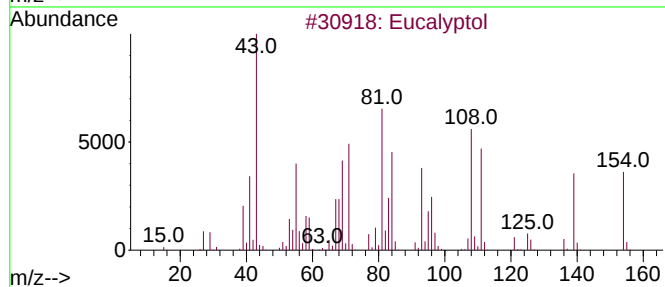
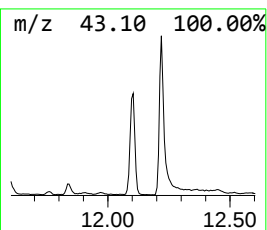
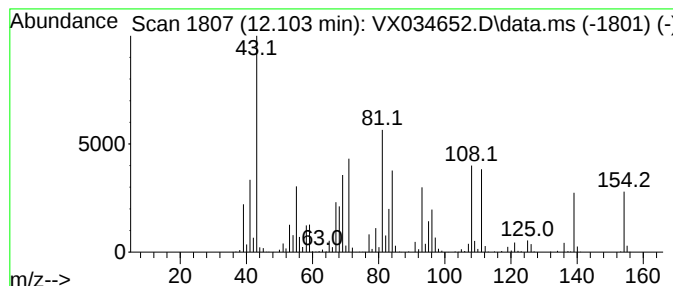
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Quant Title : SW846 8260

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

Peak Number 2 Eucalyptol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.103	42.86 ug/l	963920	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	99
2			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	59
3			Cyclohexanol, 1-methyl-4-(1-meth...	154	C10H18O	007299-40-3	37
4			7-Oxabicyclo[2.2.1]heptane, 1-me...	154	C10H18O	000470-67-7	32
5			2-Isopropyl-5-methylhex-2-enal	154	C10H18O	035158-25-9	27



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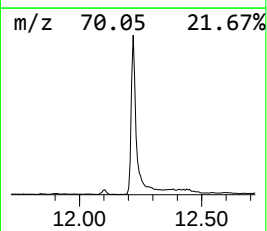
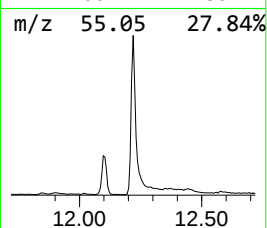
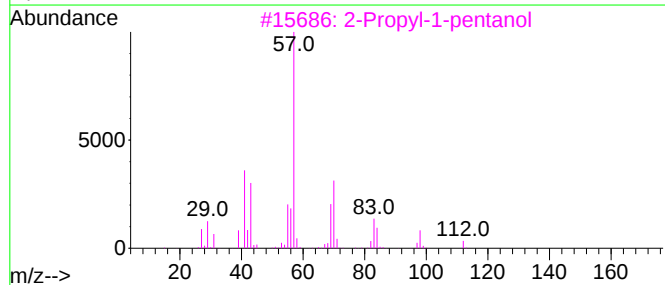
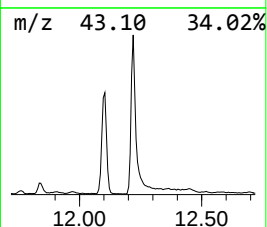
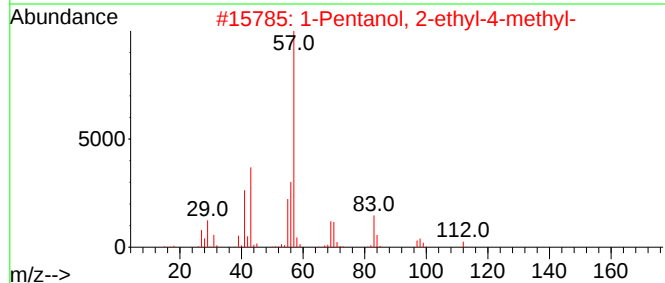
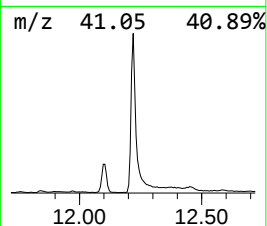
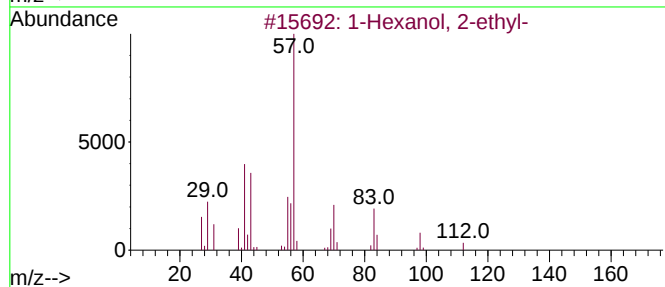
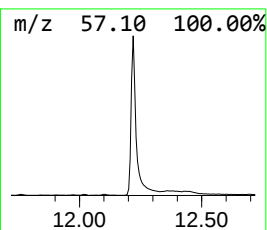
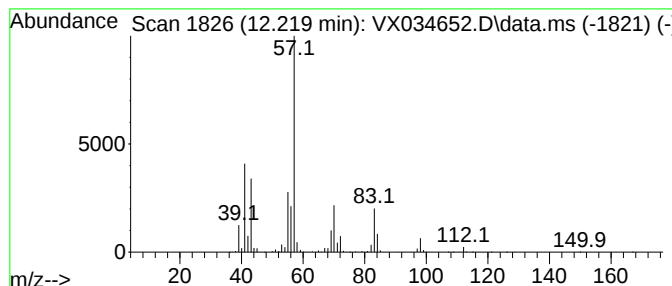
Instrument :
MSVOA_X
ClientSampleId :
215

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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD			R.T.
12.219	94.85 ug/l	2133080	1,4-Dichlorobenzene-d4			12.024
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-		130	C8H18O	000104-76-7	78
2	1-Pentanol, 2-ethyl-4-methyl-		130	C8H18O	000106-67-2	56
3	2-Propyl-1-pentanol		130	C8H18O	058175-57-8	47
4	2-Ethyl-1-hexanol, methyl ether		144	C9H20O	1000365-10-2	47
5	Octane, 3,5-dimethyl-		142	C10H22	015869-93-9	45



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Instrument :
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ClientSampleId :
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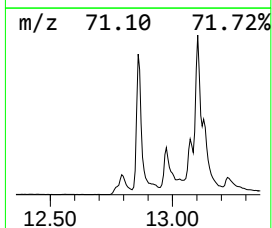
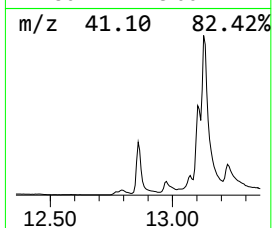
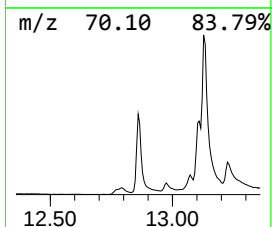
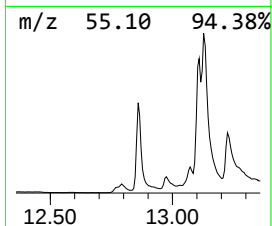
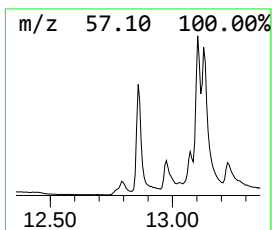
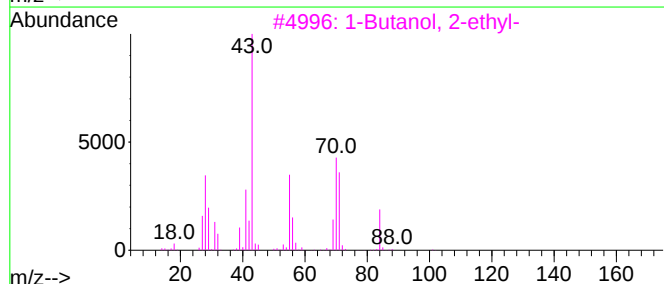
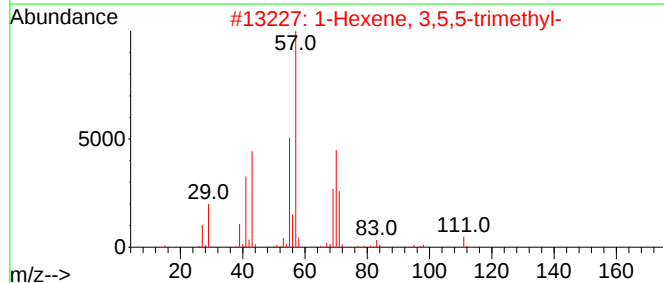
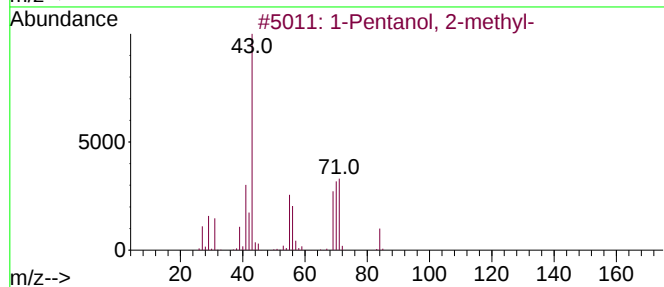
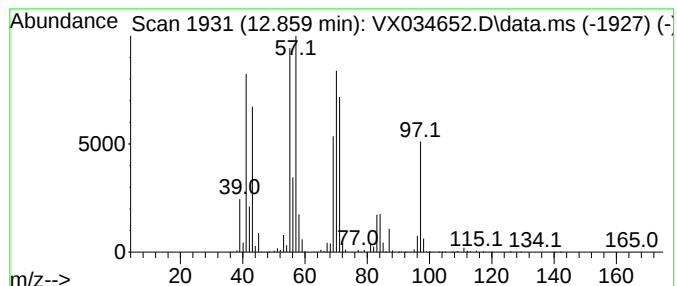
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Peak Number 4 1-Pentanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.859	189.30 ug/l	4257230	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	50
2		1-Hexene, 3,5,5-trimethyl-	126	C9H18	004316-65-8	50
3		1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	50
4		Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	002613-69-6	50
5		Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	47



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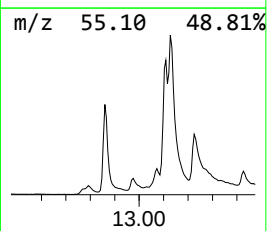
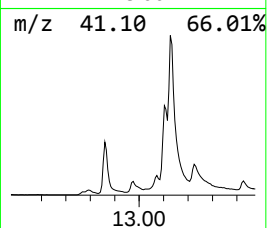
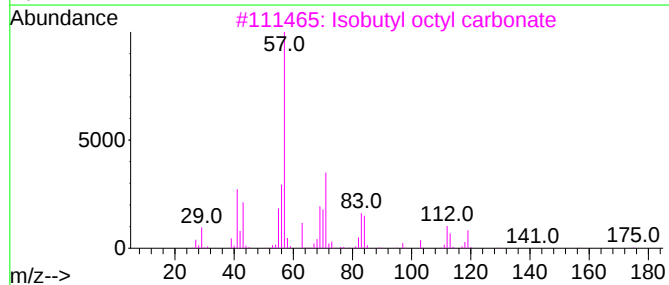
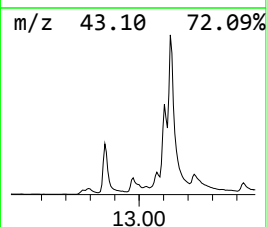
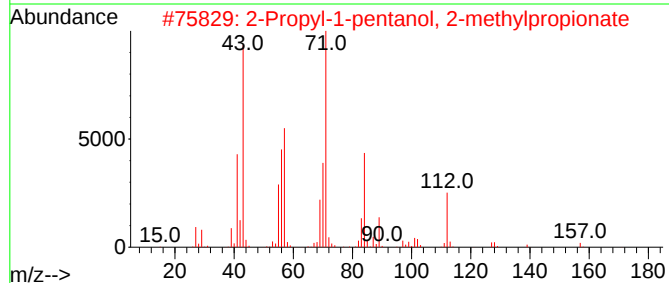
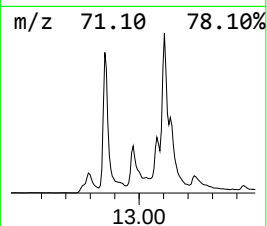
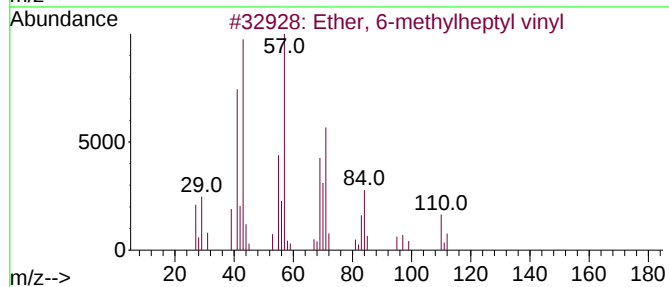
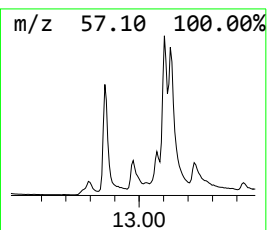
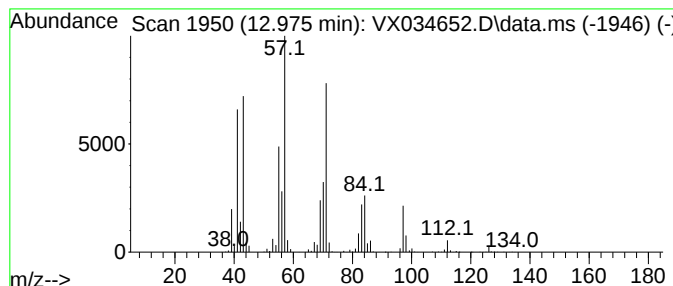
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Quant Title : SW846 8260

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

Peak Number 5 Ether, 6-methylheptyl vinyl Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.975	52.06 ug/l	1170730	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ether, 6-methylheptyl vinyl	156	C10H20O	010573-35-0	72
2			2-Propyl-1-pentanol, 2-methylpro...	200	C12H24O2	1000447-36-4	53
3			Isobutyl octyl carbonate	230	C13H26O3	1010372-74-6	52
4			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	50
5			Nonane, 2,3-dimethyl-	156	C11H24	002884-06-2	47



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215

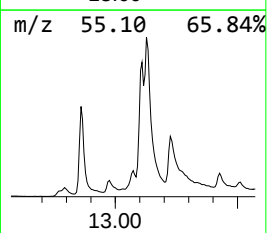
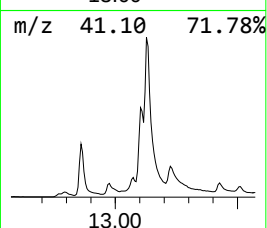
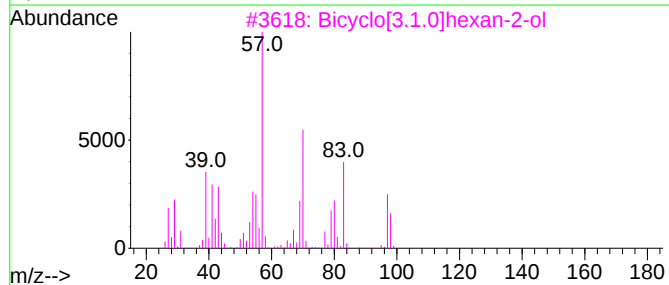
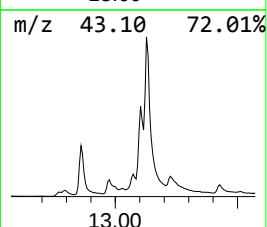
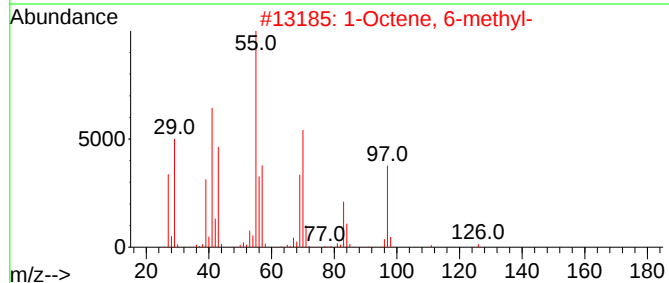
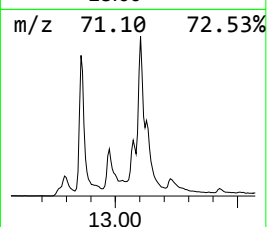
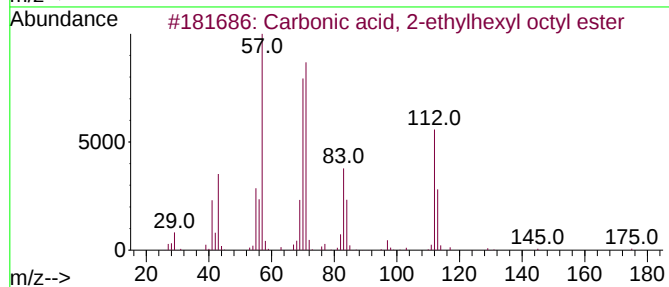
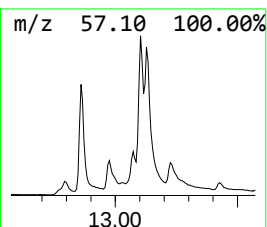
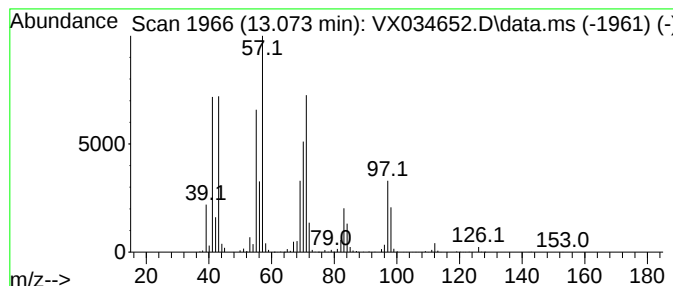
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Quant Title : SW846 8260

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

Peak Number 6 Carbonic acid, 2-ethylhexyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.073	56.08 ug/l	1261090	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, 2-ethylhexyl octy...	286	C17H34O3	1000383-13-5	59
2			1-Octene, 6-methyl-	126	C9H18	013151-10-5	55
3			Bicyclo[3.1.0]hexan-2-ol	98	C6H10O	1000194-18-6	43
4			Cycloheptane, methyl-	112	C8H16	004126-78-7	42
5			trans-1-Butyl-2-methylcyclopropane	112	C8H16	038851-70-6	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032123\
Data File : VX034652.D
Acq On : 21 Mar 2023 14:16
Operator : JC/MD
Sample : 02013-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
215

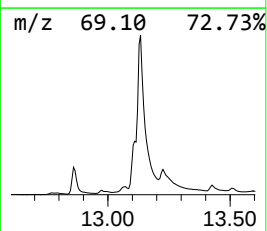
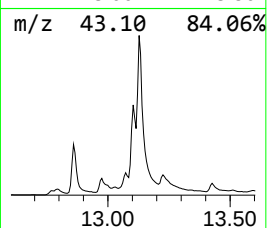
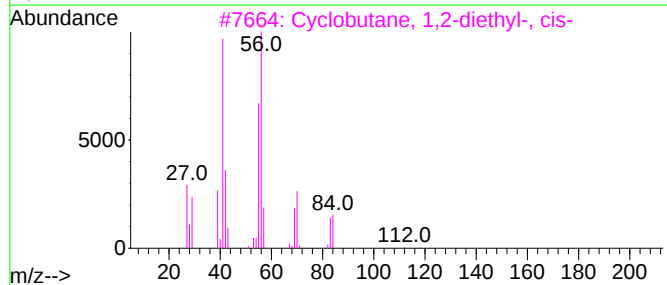
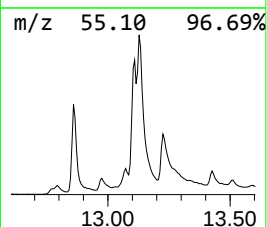
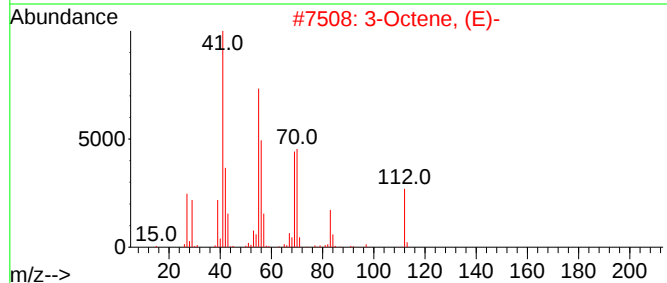
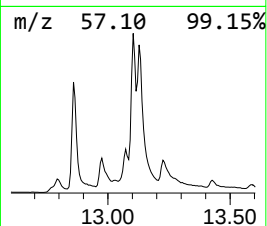
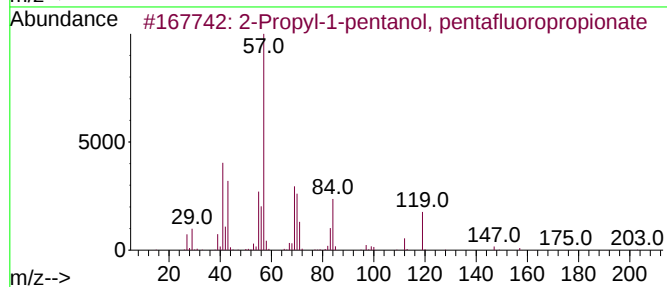
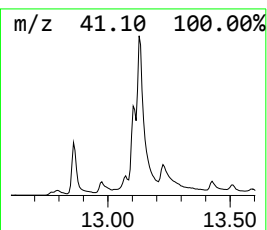
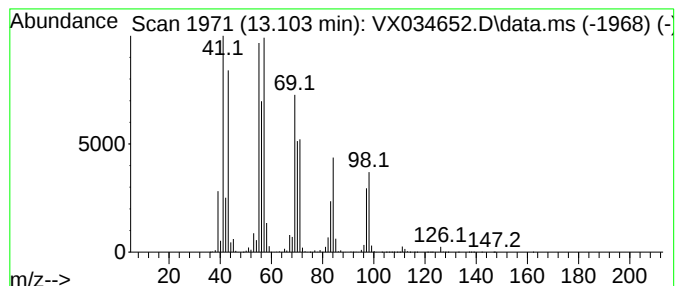
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Quant Title : SW846 8260

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

Peak Number 7 unknown13.103 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.103	256.98 ug/l	5779070	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propyl-1-pentanol, pentafluoro...	276	C11H17F5O2	1000365-51-2	47
2		3-Octene, (E)-	112	C8H16	014919-01-8	46
3		Cyclobutane, 1,2-diethyl-, cis-	112	C8H16	061141-50-2	43
4		Cyclopropane, 1,1,2,3-tetramethyl-	98	C7H14	074752-93-5	38
5		Ethanamine, N-butylidene-	99	C6H13N	001611-12-7	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032123\
Data File : VX034652.D
Acq On : 21 Mar 2023 14:16
Operator : JC/MD
Sample : 02013-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
215

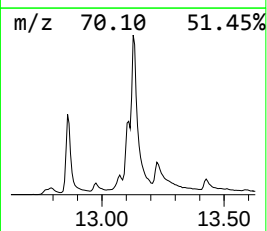
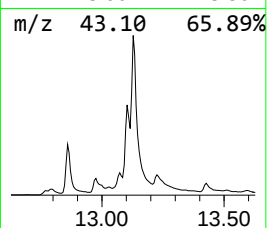
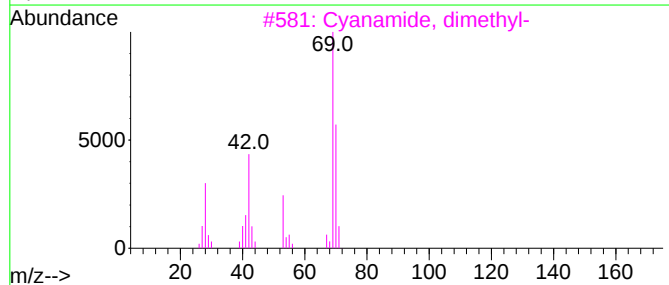
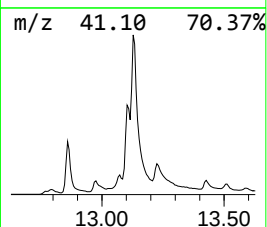
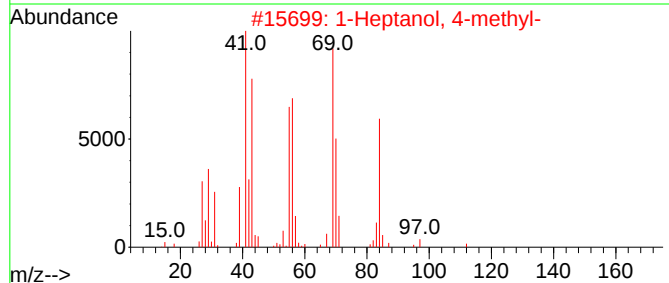
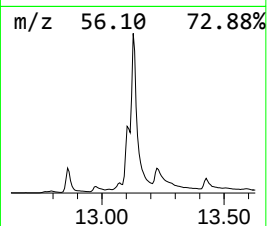
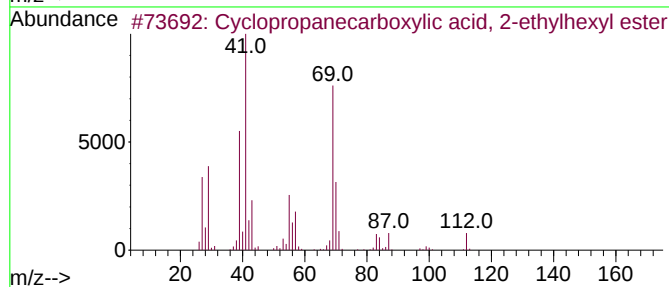
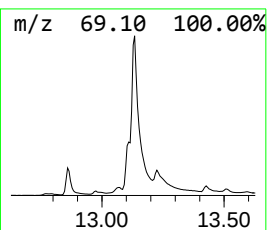
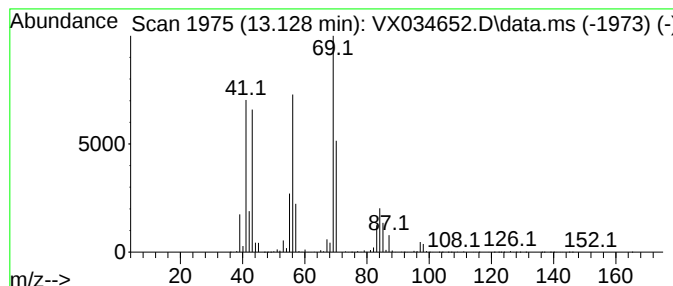
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Quant Title : SW846 8260

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

Peak Number 8 Cyclopropanecarboxylic acid... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.128	584.68 ug/l	13148800	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropanecarboxylic acid, 2-e...	198	C12H22O2	103604-31-5	50
2			1-Heptanol, 4-methyl-	130	C8H18O	000817-91-4	45
3			Cyanamide, dimethyl-	70	C3H6N2	001467-79-4	43
4			1-Decanol	158	C10H22O	000112-30-1	38
5			4-Methyl-2-hexene,c&t	98	C7H14	003404-55-5	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032123\
Data File : VX034652.D
Acq On : 21 Mar 2023 14:16
Operator : JC/MD
Sample : 02013-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
215

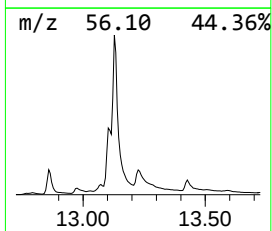
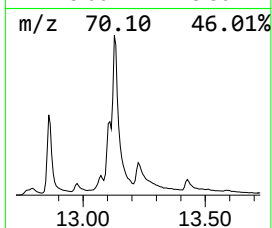
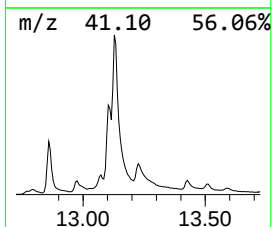
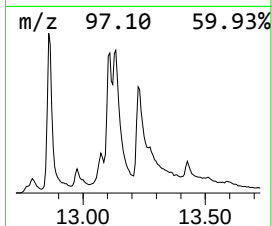
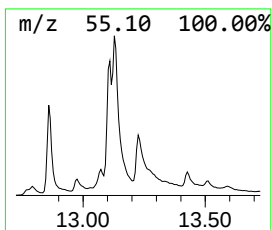
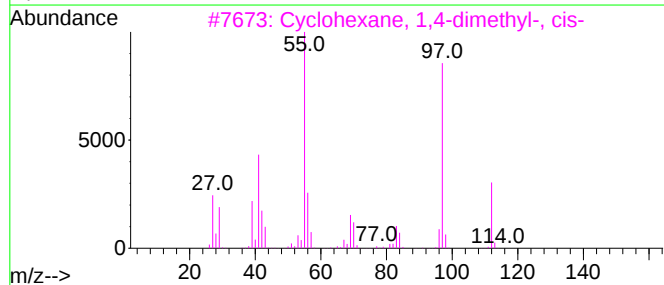
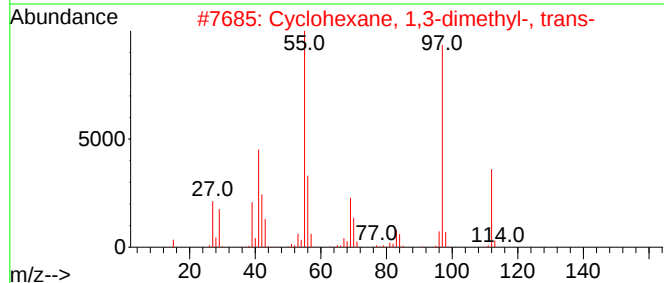
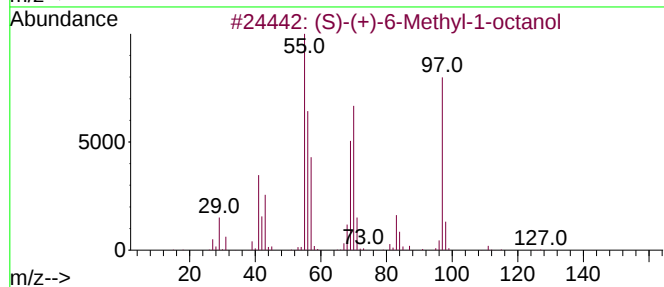
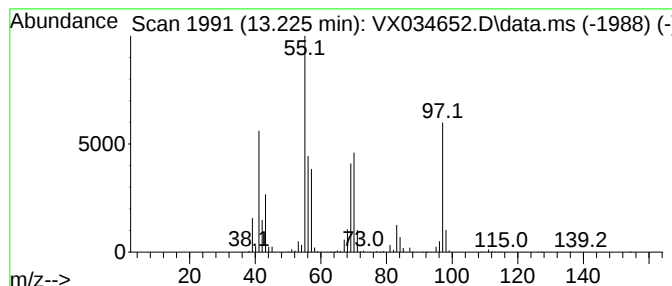
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Quant Title : SW846 8260

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

Peak Number 9 (S)-(+)-6-Methyl-1-octanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.225	139.96 ug/l	3147530	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		(S)-(+)-6-Methyl-1-octanol	144	C9H20O	110453-78-6	91
2		Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	53
3		Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	50
4		Cyclopentane, 1,2-dimethyl-3-(1-...	140	C10H20	000489-20-3	50
5		Cyclopropane, 1-methyl-2-(3-meth...	140	C10H20	062238-07-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032123\
Data File : VX034652.D
Acq On : 21 Mar 2023 14:16
Operator : JC/MD
Sample : 02013-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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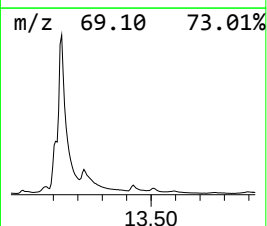
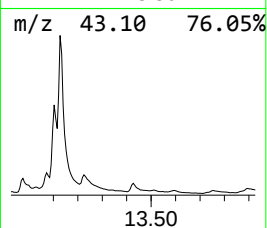
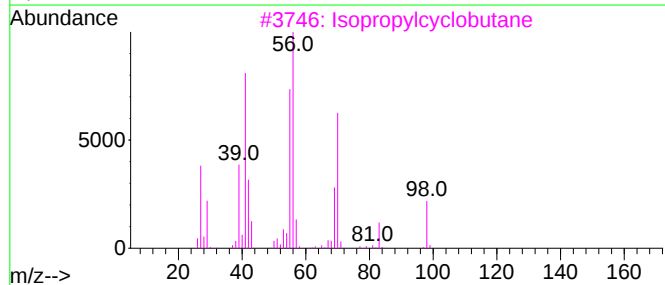
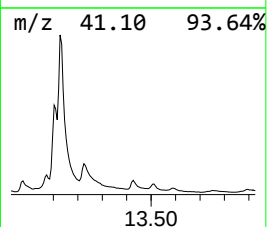
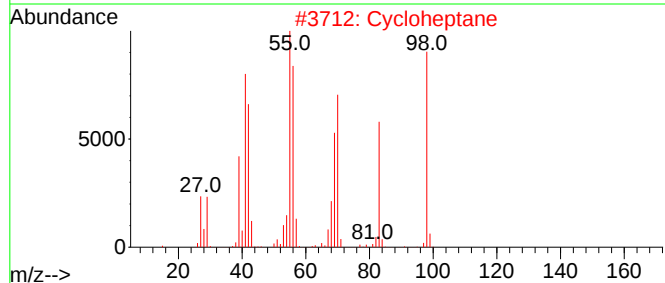
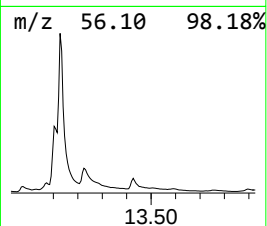
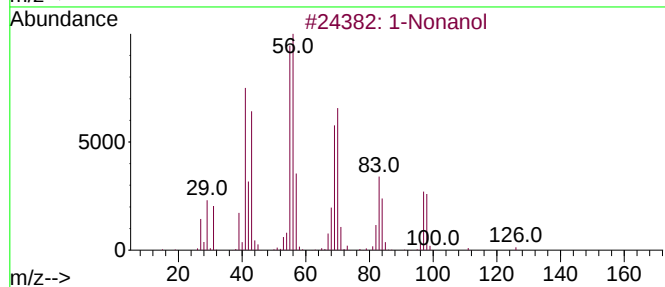
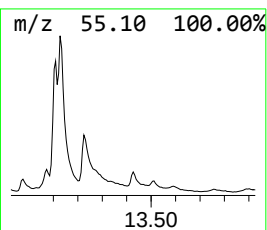
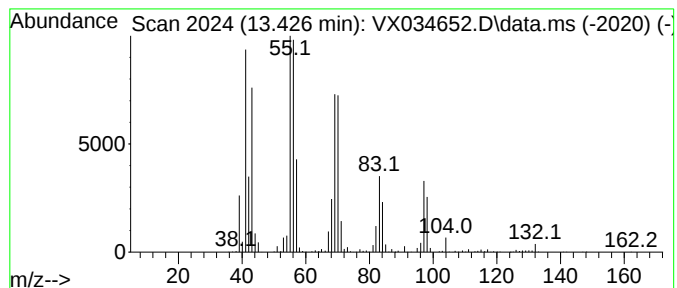
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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

Peak Number 10 1-Nonanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.426	39.29 ug/l	883523	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Nonanol	144	C9H20O	000143-08-8	91
2			Cycloheptane	98	C7H14	000291-64-5	64
3			Isopropylcyclobutane	98	C7H14	000872-56-0	62
4			Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	53
5			Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032123\
Data File : VX034652.D
Acq On : 21 Mar 2023 14:16
Operator : JC/MD
Sample : 02013-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
215

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.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	2.050	39.0	ug/l	567600	1	5.550	727430	50.0
Eucalyptol	12.103	42.9	ug/l	963920	4	12.024	1124440	50.0
1-Hexanol, 2-et...	12.219	94.8	ug/l	2133080	4	12.024	1124440	50.0
1-Pentanol, 2-m...	12.859	189.3	ug/l	4257230	4	12.024	1124440	50.0
Ether, 6-methyl...	12.975	52.1	ug/l	1170730	4	12.024	1124440	50.0
Carbonic acid, ...	13.073	56.1	ug/l	1261090	4	12.024	1124440	50.0
unknown13.103	13.103	257.0	ug/l	5779070	4	12.024	1124440	50.0
Cyclopropanecar...	13.128	584.7	ug/l	13148800	4	12.024	1124440	50.0
(S)-(+)-6-Methy...	13.225	140.0	ug/l	3147530	4	12.024	1124440	50.0
1-Nonanol	13.426	39.3	ug/l	883523	4	12.024	1124440	50.0