

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
 Data File : VX039603.D
 Acq On : 03 Jan 2024 15:36
 Operator : JC/MD
 Sample : P1002-07
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1215

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\82X121323W.M
 Title : SW846 8260

Signal : TIC: VX039603.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	18	rBV	39542	41240	1.68%	0.425%
2	1.246	22	26	34	rBV	13008	25863	1.05%	0.266%
3	2.050	153	158	166	rVB	18506	29374	1.19%	0.302%
4	2.288	192	197	205	rVB	15058	25977	1.06%	0.267%
5	2.374	205	211	225	rVB	78540	128170	5.21%	1.319%
6	2.526	229	236	249	rVB	41023	78216	3.18%	0.805%
7	2.947	295	305	319	rBV	13947	33438	1.36%	0.344%
8	4.227	504	515	529	rBV	118750	320876	13.04%	3.303%
9	4.562	562	570	581	rBV	8960	26279	1.07%	0.271%
10	5.385	694	705	720	rBV	70265	203627	8.28%	2.096%
11	5.550	720	732	748	rVB	99728	284921	11.58%	2.933%
12	5.952	788	798	812	rBV	80862	213218	8.67%	2.195%
13	6.105	815	823	836	rVV2	15939	44469	1.81%	0.458%
14	6.757	918	930	944	rBV	189441	461280	18.75%	4.749%
15	7.202	996	1003	1022	rBV	85776	198679	8.08%	2.045%
16	8.647	1233	1240	1256	rBV	410578	651603	26.49%	6.708%
17	10.055	1464	1471	1483	rBV	456976	652893	26.54%	6.721%
18	10.750	1581	1585	1594	rBV3	38667	72099	2.93%	0.742%
19	11.079	1633	1639	1645	rBV	394991	510616	20.76%	5.257%
20	11.567	1714	1719	1733	rBV	2015594	2460190	100.00%	25.327%
21	11.683	1733	1738	1746	rVB	187082	213965	8.70%	2.203%
22	11.823	1756	1761	1767	rBV	456046	562258	22.85%	5.788%
23	11.884	1767	1771	1779	rVV	118286	157613	6.41%	1.623%
24	11.988	1779	1788	1790	rVV	111720	164060	6.67%	1.689%
25	12.018	1790	1793	1801	rVB	488154	650094	26.42%	6.693%
26	12.097	1801	1806	1812	rVB	91295	124266	5.05%	1.279%
27	12.213	1820	1825	1836	rBV	433563	583952	23.74%	6.012%
28	12.305	1836	1840	1851	rVB3	22029	48715	1.98%	0.502%
29	12.524	1871	1876	1885	rBV5	15582	27051	1.10%	0.278%
30	13.140	1971	1977	1985	rBV	96187	165495	6.73%	1.704%
31	13.213	1985	1989	1999	rVB2	52427	78989	3.21%	0.813%
32	13.579	2042	2049	2052	rBV5	18284	33042	1.34%	0.340%
33	13.676	2058	2065	2069	rBV	65281	78762	3.20%	0.811%
34	13.731	2069	2074	2078	rBV	119654	168497	6.85%	1.735%
35	13.774	2078	2081	2086	rVB2	26851	36630	1.49%	0.377%
36	14.140	2136	2141	2146	rVB	22153	27240	1.11%	0.280%

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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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Title : SW846 8260

37	15.133	2297	2304	2310	rBV3	13880	26491	1.08%	0.273%
38	15.487	2357	2362	2371	rBV3	15977	29568	1.20%	0.304%
39	15.670	2386	2392	2402	rBV2	16741	30785	1.25%	0.317%
40	15.969	2434	2441	2447	rBV3	24644	43071	1.75%	0.443%

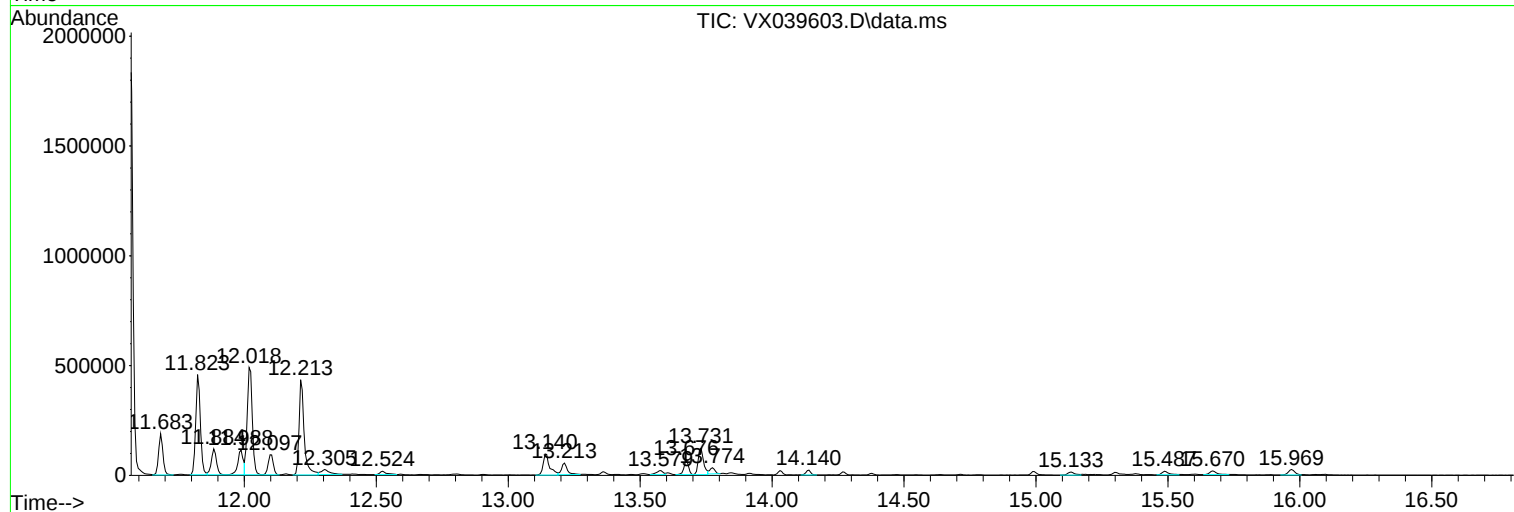
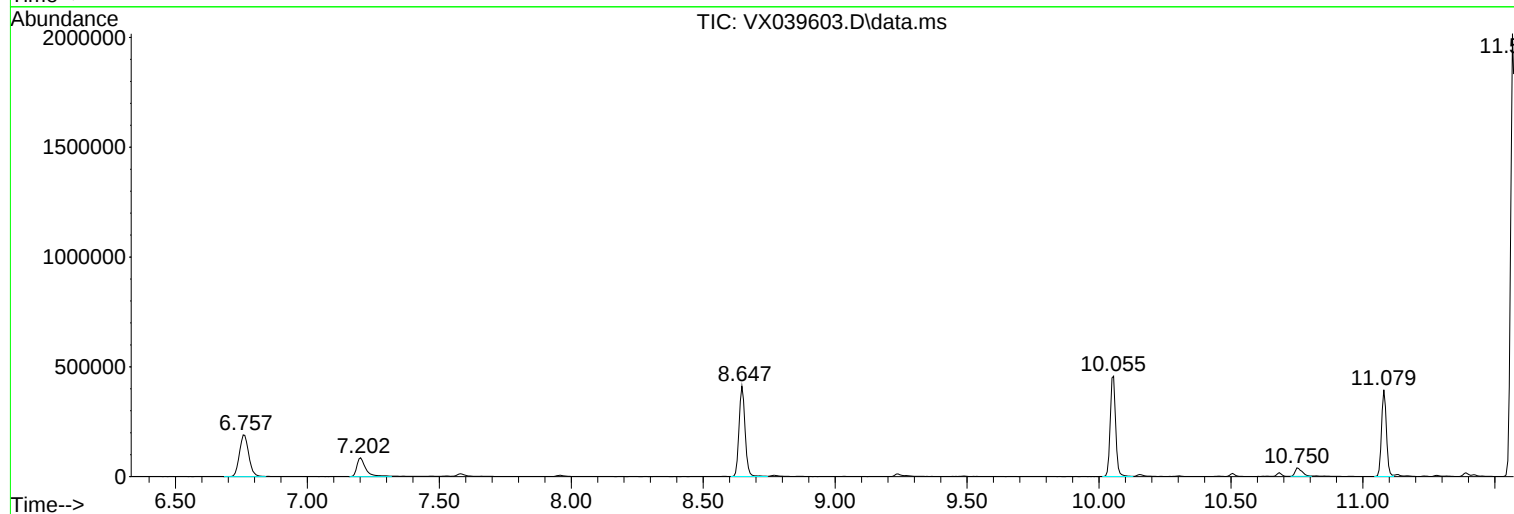
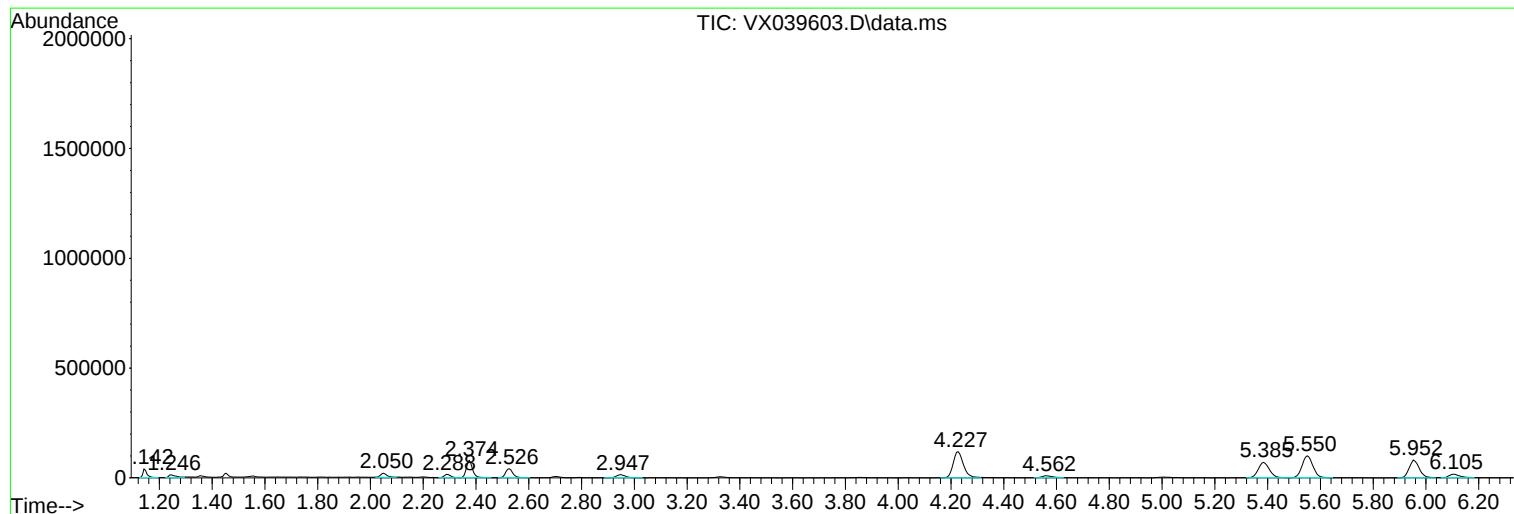
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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



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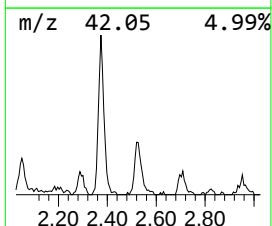
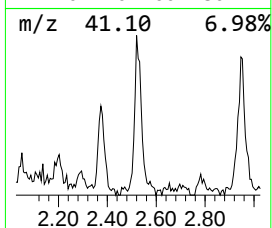
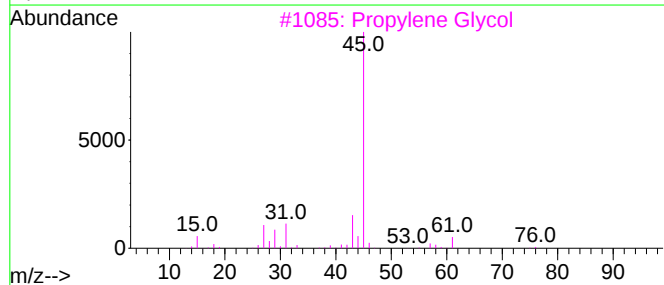
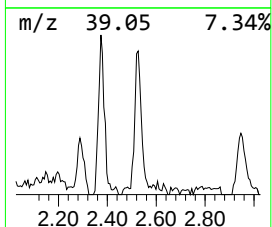
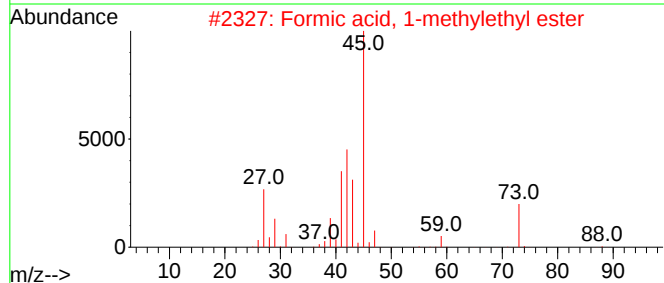
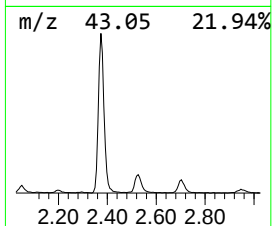
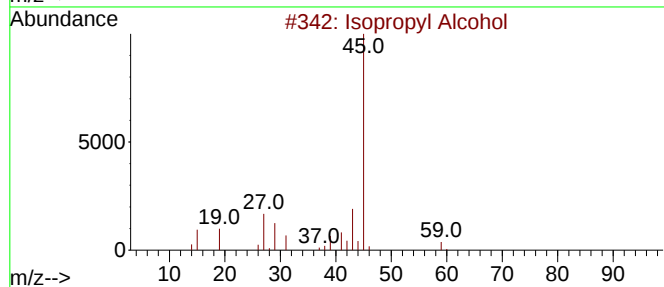
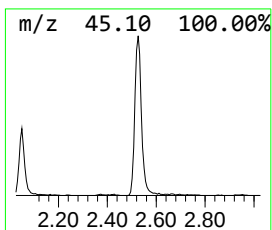
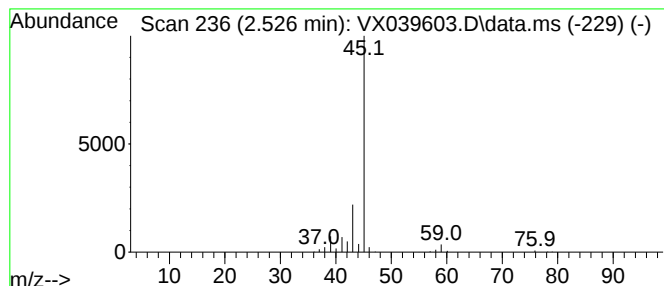
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.526	13.73 ug/l	78216	Pentafluorobenzene	5.550

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2		Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	40
3		Propylene Glycol	76	C3H8O2	000057-55-6	9
4		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
5		2-Pentanol	88	C5H12O	006032-29-7	9



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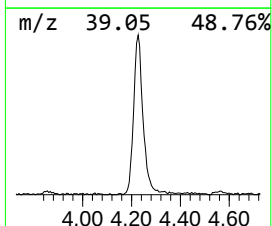
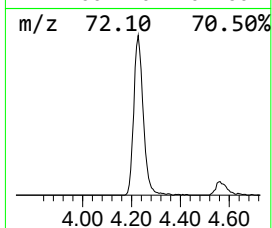
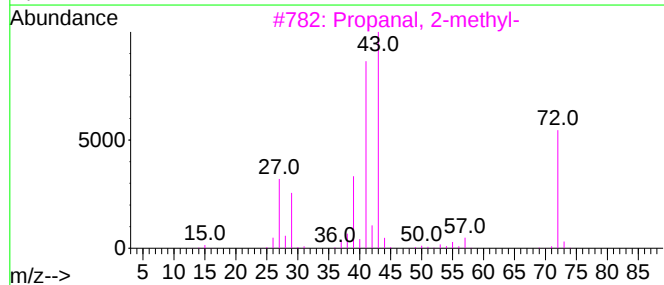
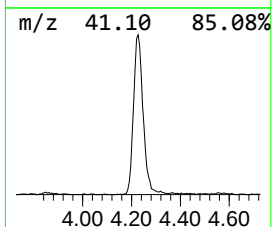
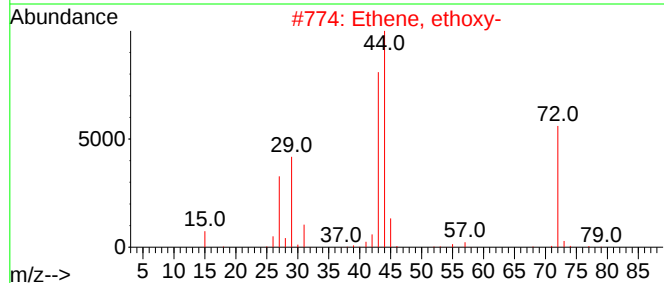
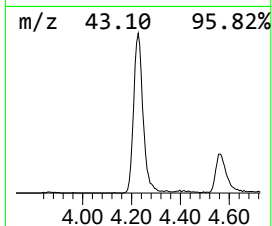
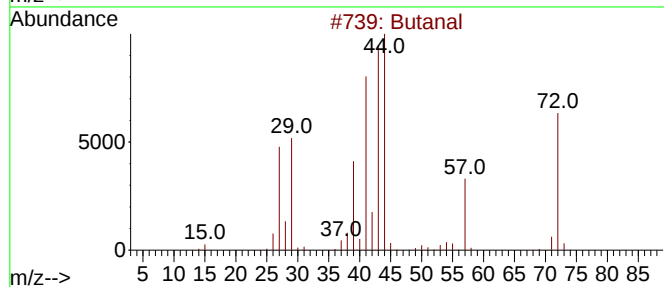
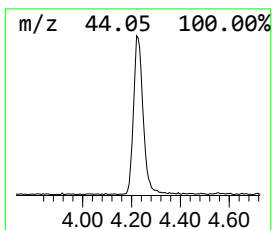
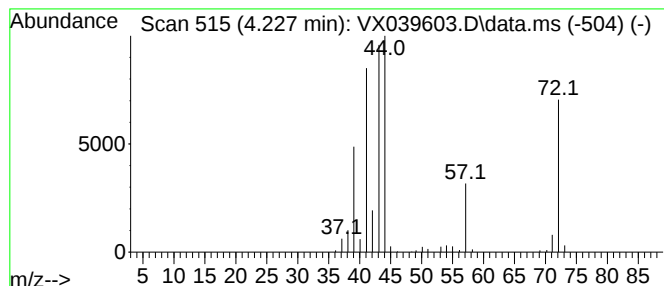
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Peak Number 2 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	56.31 ug/l	320876	Pentafluorobenzene	5.550

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanal	72	C4H8O	000123-72-8	94
2		Ethene, ethoxy-	72	C4H8O	000109-92-2	49
3		Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
4		2-Propanone, hydrazone	72	C3H8N2	005281-20-9	27
5		Methacrolein	70	C4H6O	000078-85-3	27



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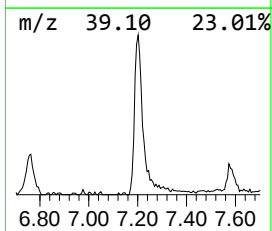
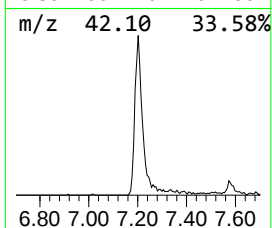
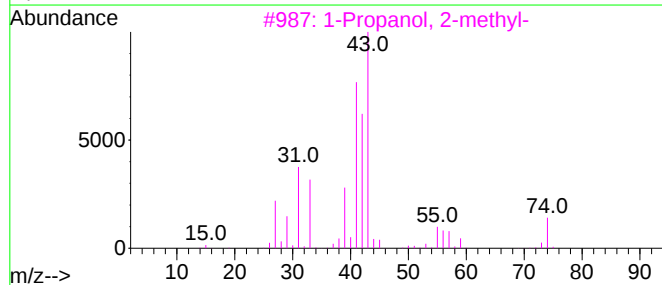
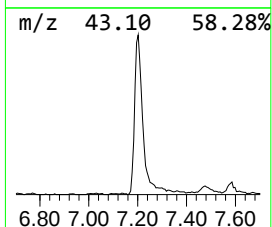
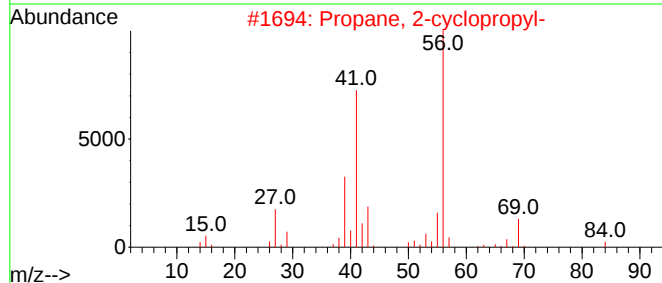
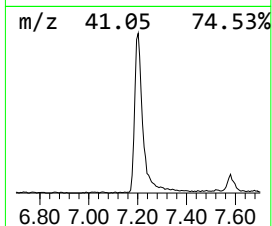
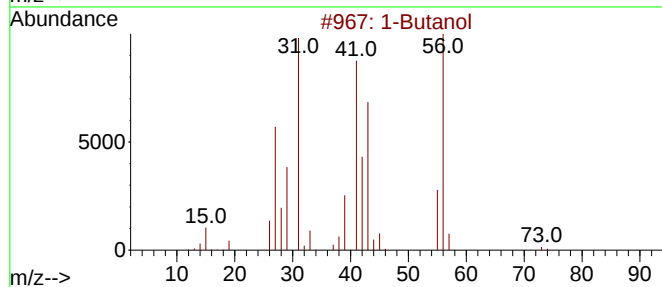
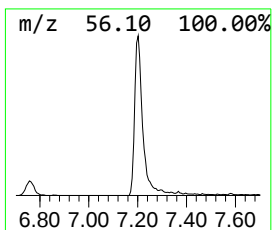
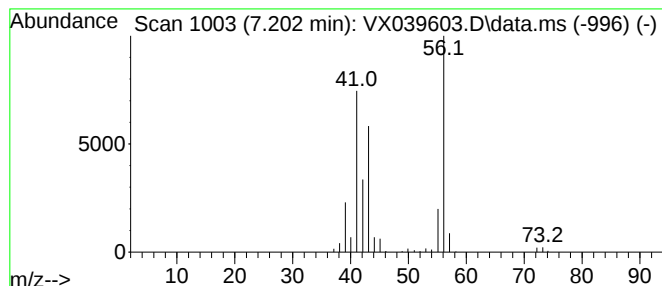
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Butanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.202	21.54 ug/l	198679	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	91
2			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	39
3			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
4			Oxetane, 2,3,4-trimethyl-, (2.al...	100	C6H12O	032347-12-9	9
5			2-Butene, (Z)-	56	C4H8	000590-18-1	9



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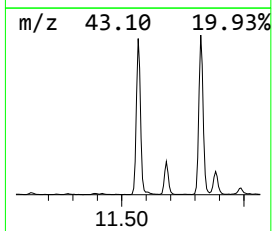
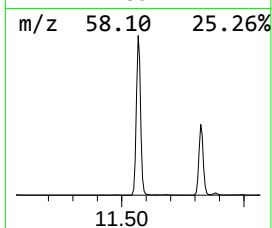
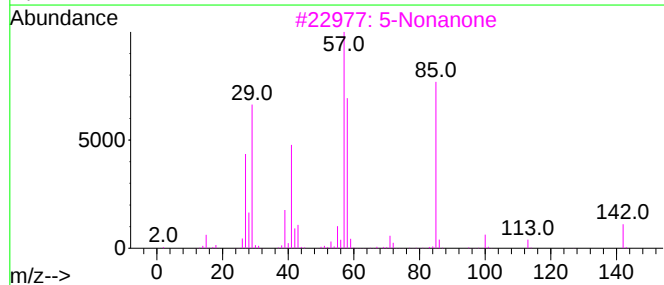
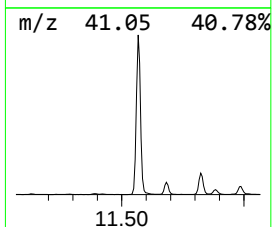
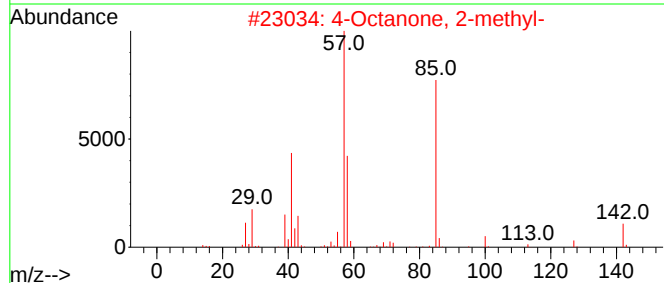
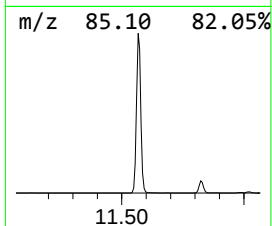
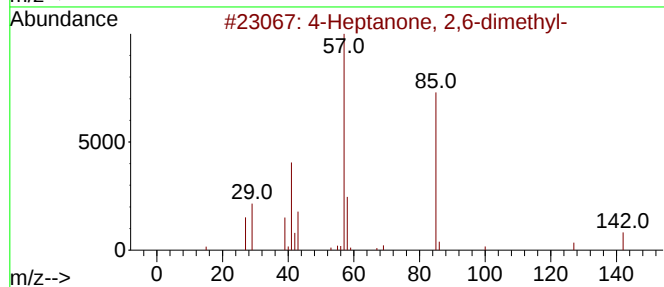
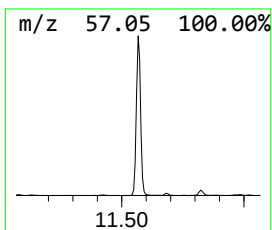
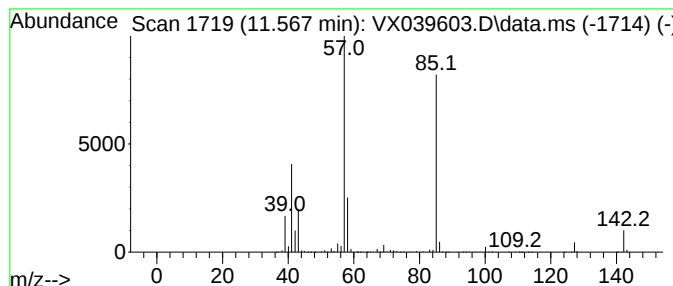
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TIC Integration Parameters: LSCINT.P

Peak Number 4 4-Heptanone, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.567	189.22 ug/l	2460190	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	94
2			4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	80
3			5-Nonanone	142	C9H18O	000502-56-7	64
4			t-Butyl isobutyl ketone	142	C9H18O	014705-50-1	59
5			3-Buten-2-ol, 2,3-dimethyl-	100	C6H12O	010473-13-9	50



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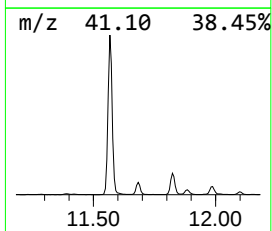
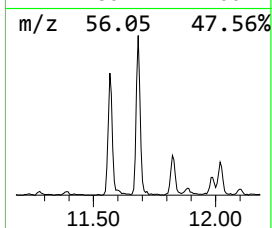
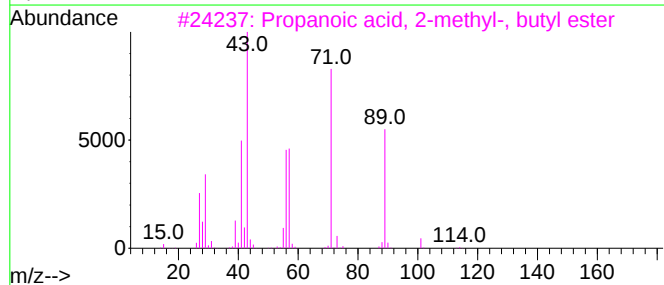
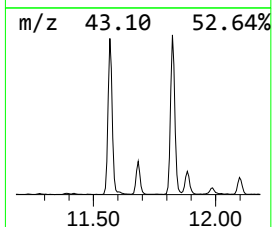
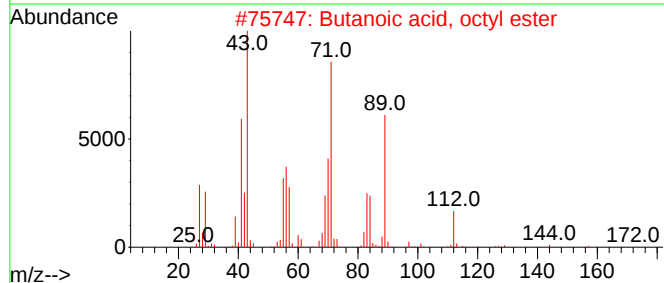
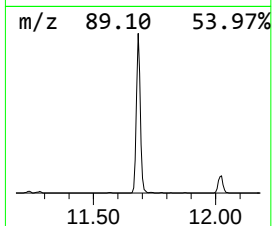
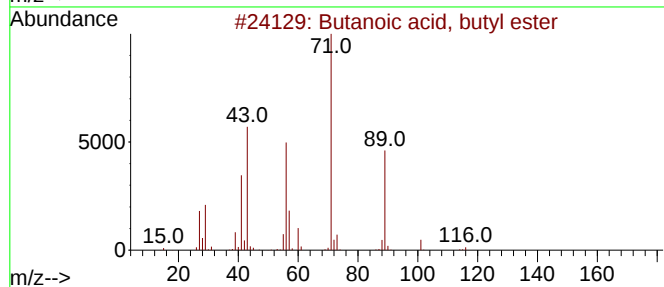
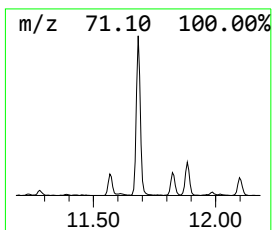
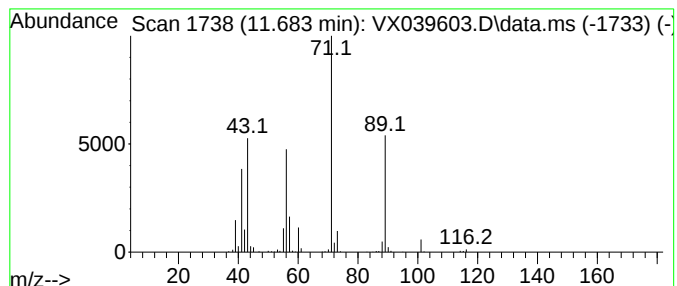
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

Peak Number 5 Butanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.683	16.46 ug/l	213965	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2			Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	72
3			Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	72
4			Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	72
5			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039603.D
Acq On : 03 Jan 2024 15:36
Operator : JC/MD
Sample : P1002-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1215

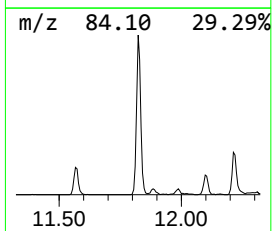
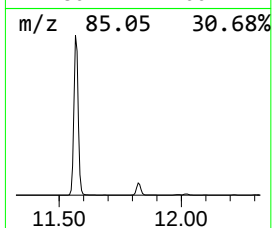
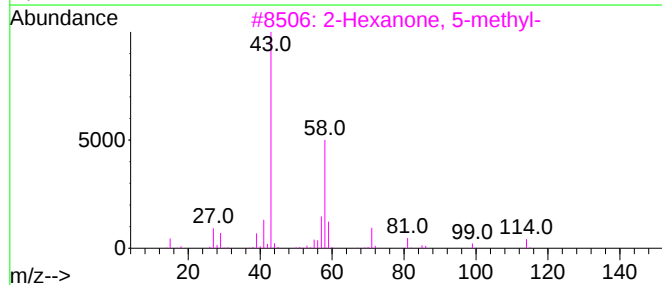
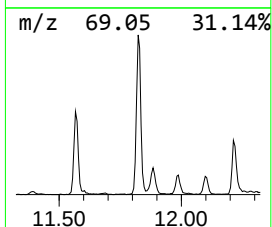
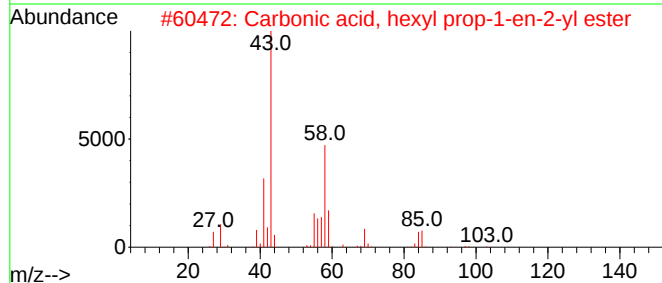
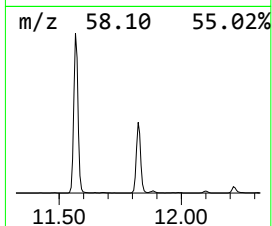
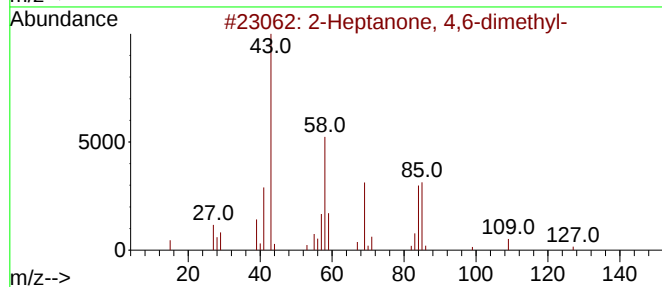
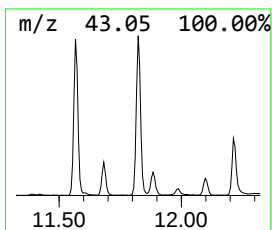
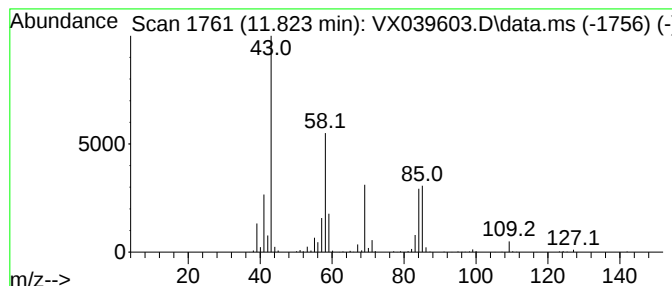
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Quant Title : SW846 8260

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

Peak Number 6 2-Heptanone, 4,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.823	43.24 ug/l	562258	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone, 4,6-dimethyl-	142	C9H18O	019549-80-5	90		
2	Carbonic acid, hexyl prop-1-en-2...	186	C10H18O3	1000382-54-2	64		
3	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	50		
4	Hexane, 3-ethyl-	114	C8H18	000619-99-8	43		
5	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	43		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039603.D
Acq On : 03 Jan 2024 15:36
Operator : JC/MD
Sample : P1002-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1215

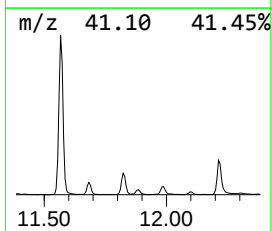
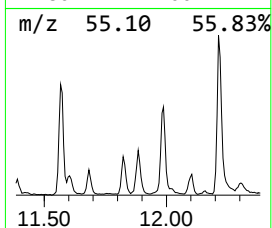
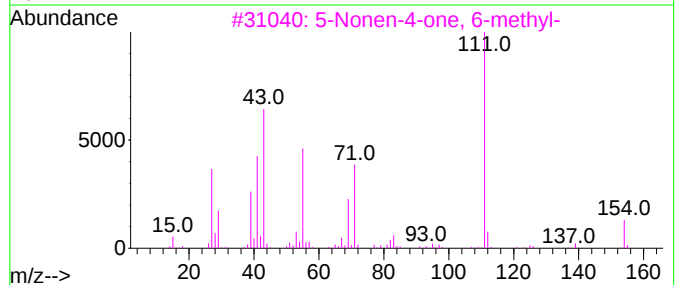
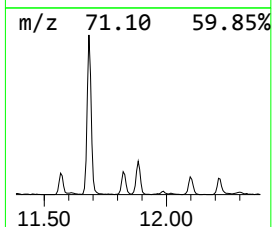
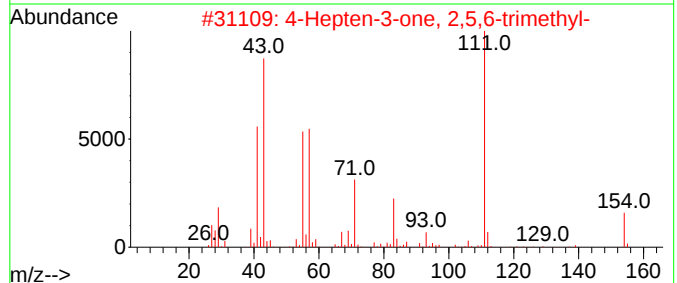
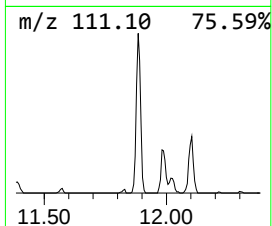
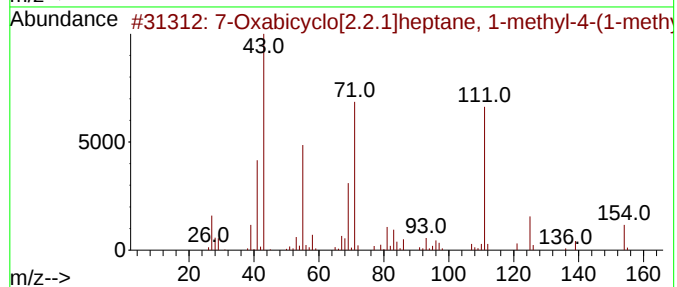
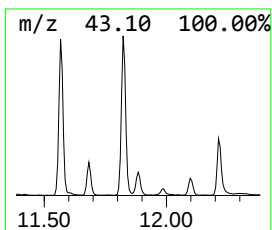
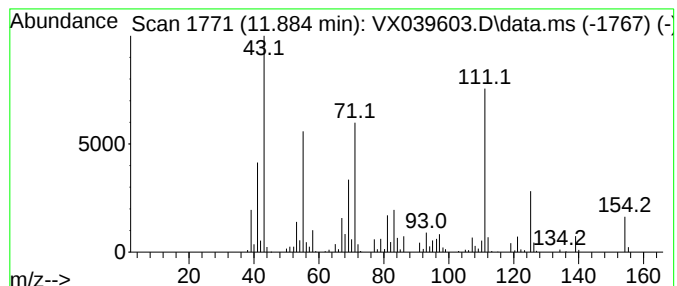
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Quant Title : SW846 8260

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

Peak Number 7 7-Oxabicyclo[2.2.1]heptane,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.884	12.12 ug/l	157613	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Oxabicyclo[2.2.1]heptane, 1-me...	154	C10H18O	000470-67-7	81
2			4-Hepten-3-one, 2,5,6-trimethyl-	154	C10H18O	016466-21-0	53
3			5-Nonen-4-one, 6-methyl-	154	C10H18O	007036-98-8	50
4			cis-1-Hydroxybicyclo[4.4.0]decane	154	C10H18O	003574-58-1	43
5			1,2-Propanedione, 1-(2-thienyl)-	154	C7H6O2S	013678-69-8	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039603.D
Acq On : 03 Jan 2024 15:36
Operator : JC/MD
Sample : P1002-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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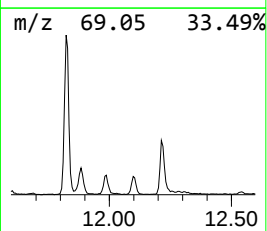
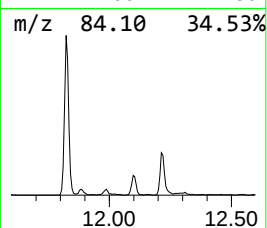
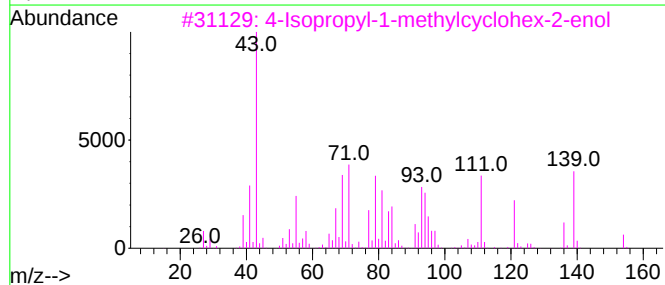
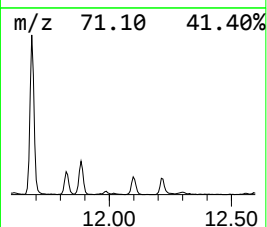
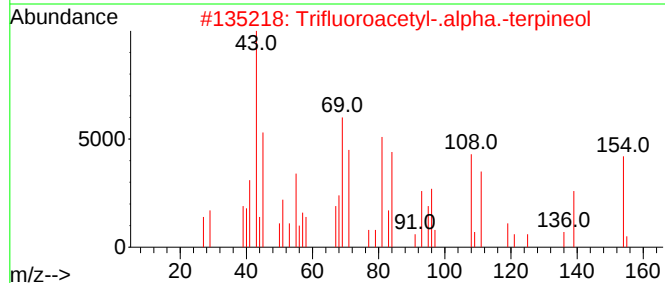
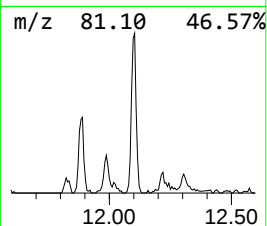
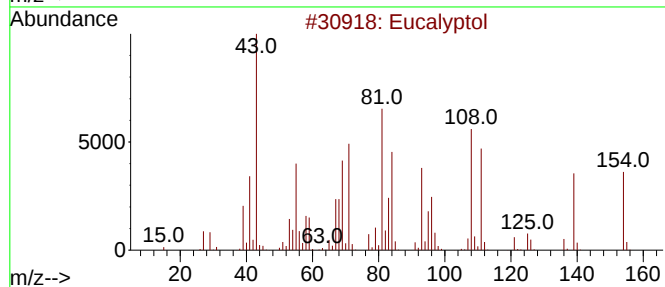
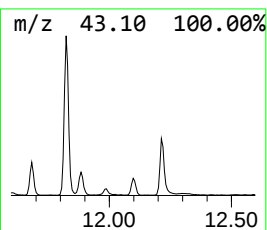
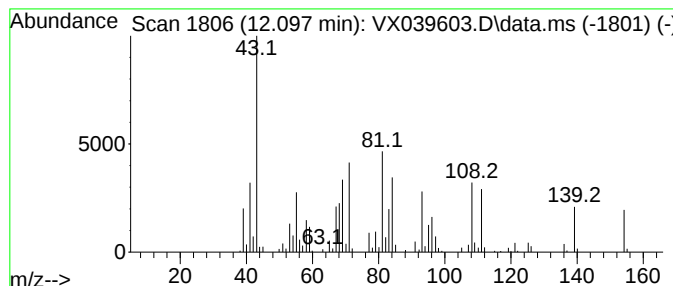
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Quant Title : SW846 8260

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

Peak Number 8 Eucalyptol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.097	9.56 ug/l	124266	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	96
2			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	40
3			4-Isopropyl-1-methylcyclohex-2-enol	154	C10H18O	000619-62-5	37
4			2-Isopropyl-5-methylhex-2-enal	154	C10H18O	035158-25-9	35
5			7-Decen-2-one	154	C10H18O	035194-33-3	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039603.D
Acq On : 03 Jan 2024 15:36
Operator : JC/MD
Sample : P1002-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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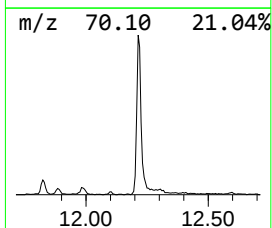
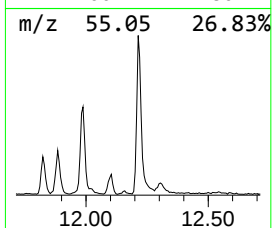
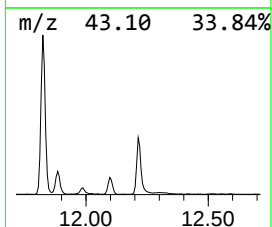
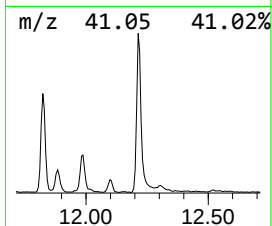
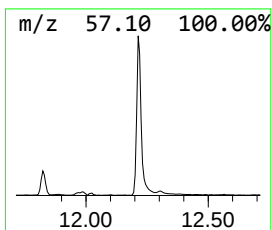
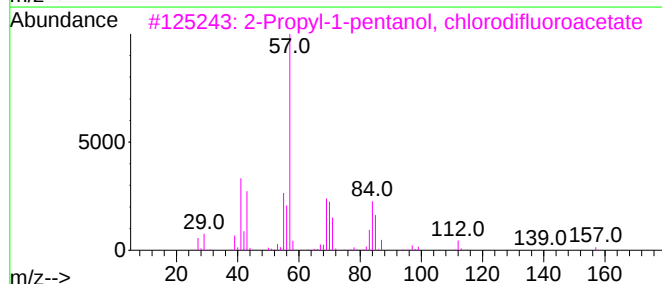
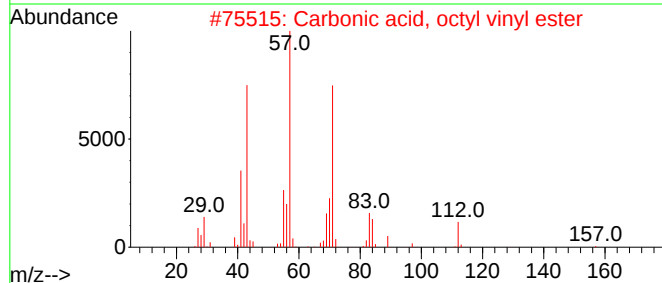
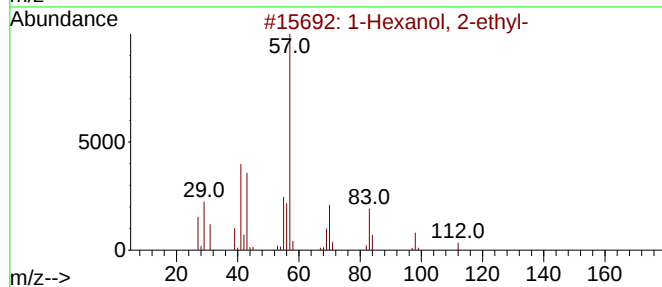
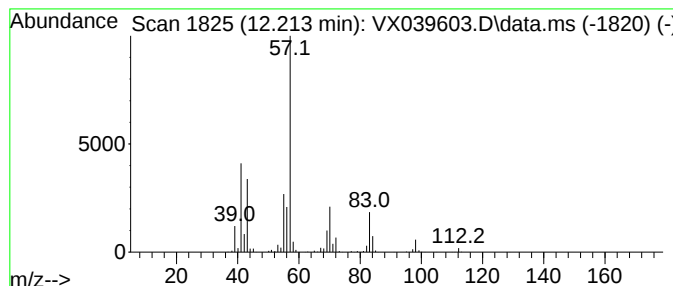
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Quant Title : SW846 8260

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

Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.213	44.91 ug/l	583952	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			Carbonic acid, octyl vinyl ester	200	C11H20O3	1000383-25-5	64
3			2-Propyl-1-pentanol, chlorodiflu...	242	C10H17ClF2O2	1000447-27-3	53
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
5			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039603.D
Acq On : 03 Jan 2024 15:36
Operator : JC/MD
Sample : P1002-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

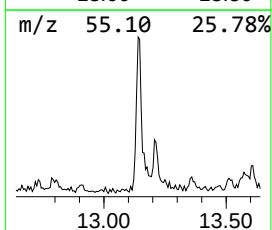
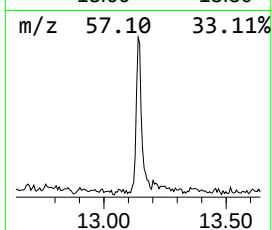
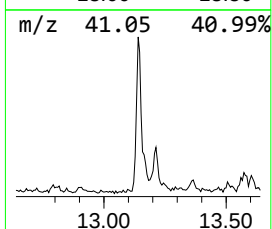
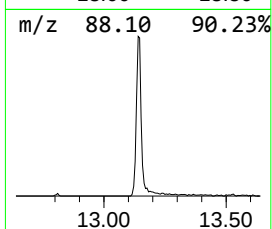
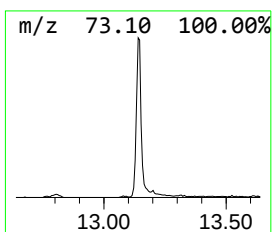
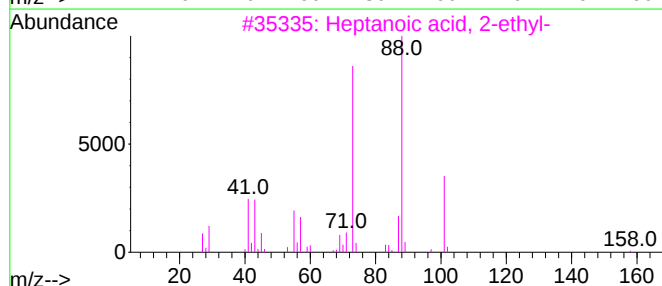
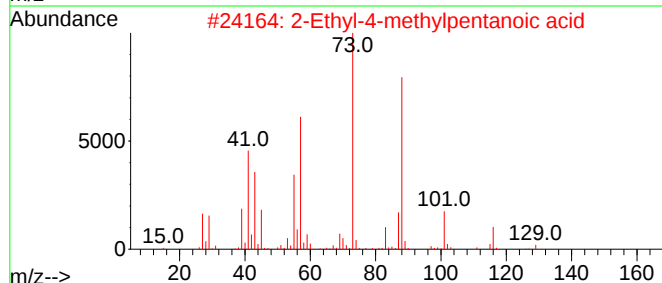
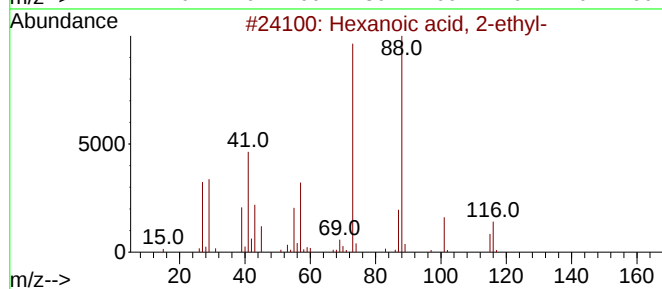
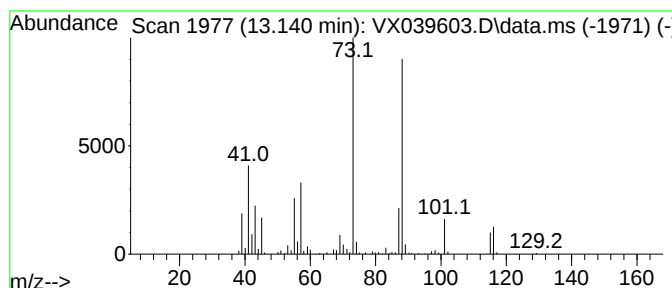
Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

Peak Number 10 Hexanoic acid, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.140	12.73 ug/l	165495	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	50
3	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	42
4	Methyl-4-deoxy-2,3-di-O-methyl.b...	218	C9H14O6	1000312-09-9	42
5	Acetic acid, diethyl-	116	C6H12O2	000088-09-5	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039603.D
Acq On : 03 Jan 2024 15:36
Operator : JC/MD
Sample : P1002-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.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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Butanal	4.227	56.3	ug/l	320876	1	5.550	284921	50.0
1-Butanol	7.202	21.5	ug/l	198679	2	6.757	461280	50.0
4-Heptanone, 2,...	11.567	189.2	ug/l	2460190	4	12.024	650094	50.0
Butanoic acid, ...	11.683	16.5	ug/l	213965	4	12.024	650094	50.0
2-Heptanone, 4,...	11.823	43.2	ug/l	562258	4	12.024	650094	50.0
7-Oxabicyclo[2....	11.884	12.1	ug/l	157613	4	12.024	650094	50.0
Eucalyptol	12.097	9.6	ug/l	124266	4	12.024	650094	50.0
1-Hexanol, 2-et...	12.213	44.9	ug/l	583952	4	12.024	650094	50.0
Hexanoic acid, ...	13.140	12.7	ug/l	165495	4	12.024	650094	50.0