

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110923\
 Data File : VX038674.D
 Acq On : 09 Nov 2023 12:46
 Operator : JC/MD
 Sample : 05287-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 50188

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\82X110723W.M
 Title : SW846 8260

Signal : TIC: VX038674.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.368	41	46	52	rVB	81841	94037	2.21%	0.407%
2	1.752	103	109	117	rBV	41122	54313	1.28%	0.235%
3	2.057	151	159	173	rBV	2449673	4034475	95.01%	17.451%
4	2.215	181	185	194	rVB	41539	65712	1.55%	0.284%
5	2.374	206	211	224	rVB	191887	312635	7.36%	1.352%
6	2.526	229	236	244	rBV	35531	67397	1.59%	0.292%
7	2.752	268	273	282	rVB	23263	43484	1.02%	0.188%
8	3.111	321	332	347	rBV	108109	254766	6.00%	1.102%
9	4.556	562	569	581	rBV	29884	85781	2.02%	0.371%
10	4.709	581	594	617	rVB	185868	531529	12.52%	2.299%
11	5.385	693	705	716	rBV	171358	502661	11.84%	2.174%
12	5.550	723	732	751	rVB	268916	777017	18.30%	3.361%
13	5.958	789	799	804	rBV	162510	415247	9.78%	1.796%
14	6.038	804	812	836	rVV	743475	2016028	47.48%	8.720%
15	6.763	921	931	947	rBV	407646	998092	23.51%	4.317%
16	7.452	1038	1044	1062	rBV	118353	247349	5.83%	1.070%
17	8.647	1234	1240	1246	rBV	870755	1364846	32.14%	5.903%
18	8.720	1246	1252	1268	rVB	2692929	4246291	100.00%	18.367%
19	10.055	1465	1471	1489	rBV	931233	1314470	30.96%	5.686%
20	10.195	1489	1494	1505	rVV	242660	326451	7.69%	1.412%
21	10.299	1505	1511	1526	rVB	767051	1047321	24.66%	4.530%
22	10.640	1562	1567	1583	rVB	399171	523346	12.32%	2.264%
23	11.079	1634	1639	1651	rVB	887550	1123749	26.46%	4.861%
24	11.378	1682	1688	1696	rVV	84383	153664	3.62%	0.665%
25	11.451	1696	1700	1711	rVB	43171	58436	1.38%	0.253%
26	11.616	1721	1727	1733	rBV	40992	53684	1.26%	0.232%
27	11.750	1745	1749	1756	rVB	181570	224979	5.30%	0.973%
28	12.018	1788	1793	1800	rBV	1182733	1525428	35.92%	6.598%
29	12.085	1800	1804	1811	rVB	67068	86590	2.04%	0.375%
30	12.244	1820	1830	1838	rBV3	63102	114739	2.70%	0.496%
31	13.292	1993	2002	2007	rBV2	48850	71030	1.67%	0.307%
32	13.774	2076	2081	2088	rVB	145355	187726	4.42%	0.812%
33	14.225	2149	2155	2159	rBV3	21750	44464	1.05%	0.192%
34	14.634	2215	2222	2226	rBV2	55626	94483	2.23%	0.409%
35	15.182	2307	2312	2320	rVB2	30961	57131	1.35%	0.247%

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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

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110723W.M
Title : SW846 8260

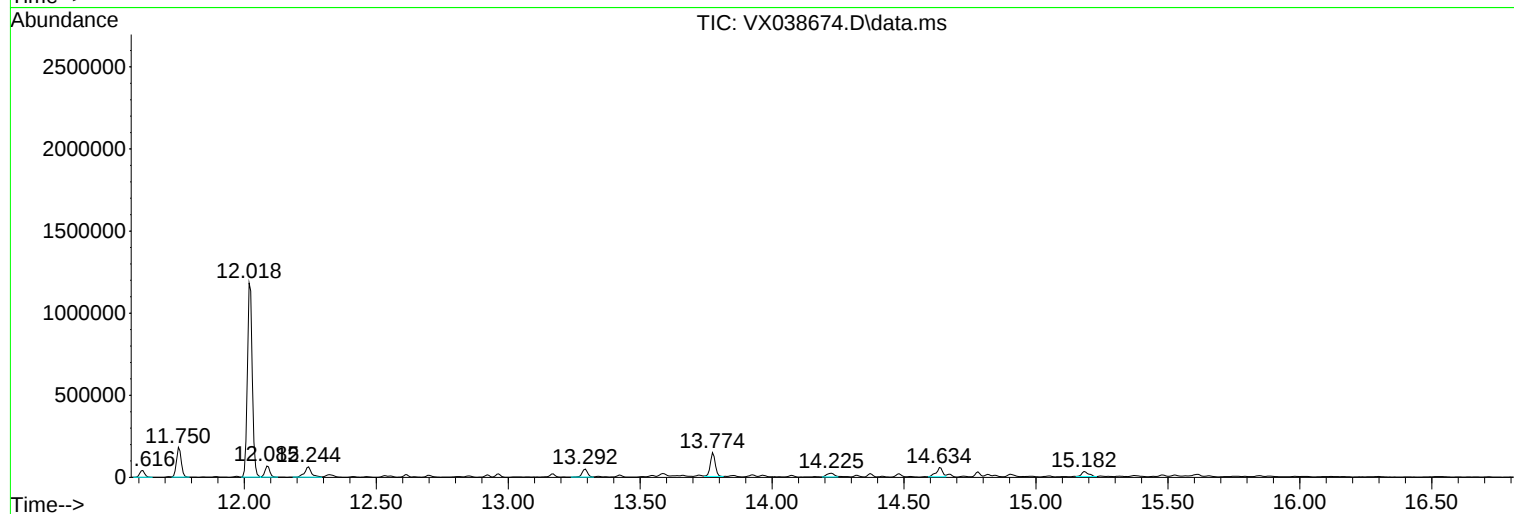
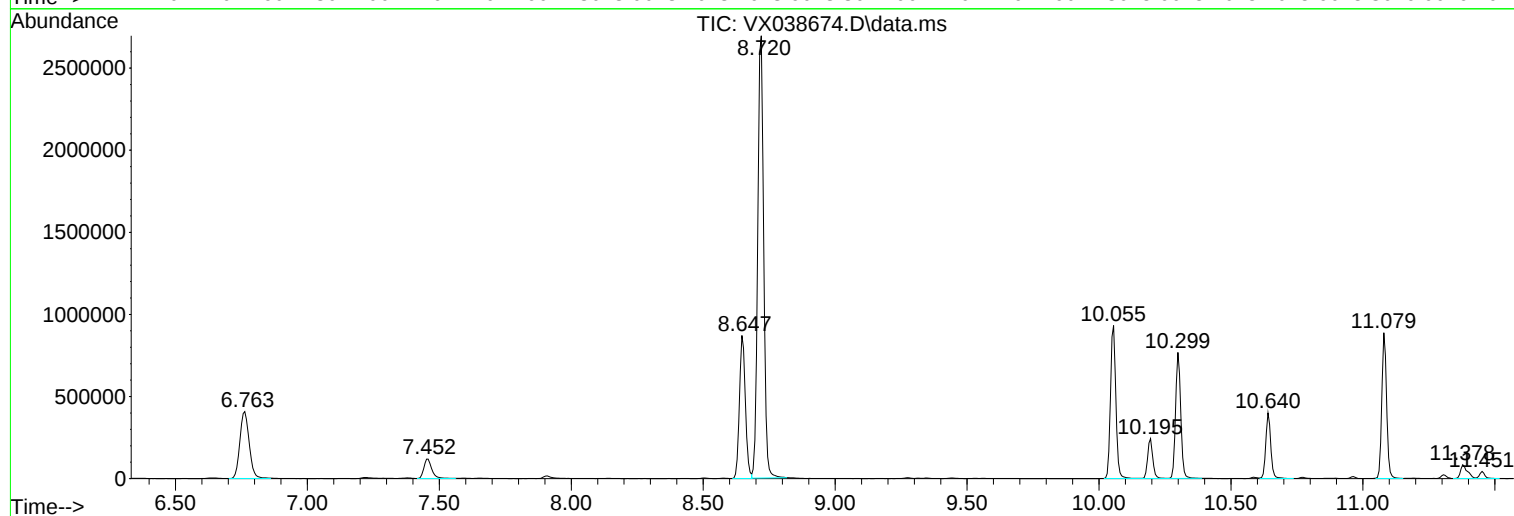
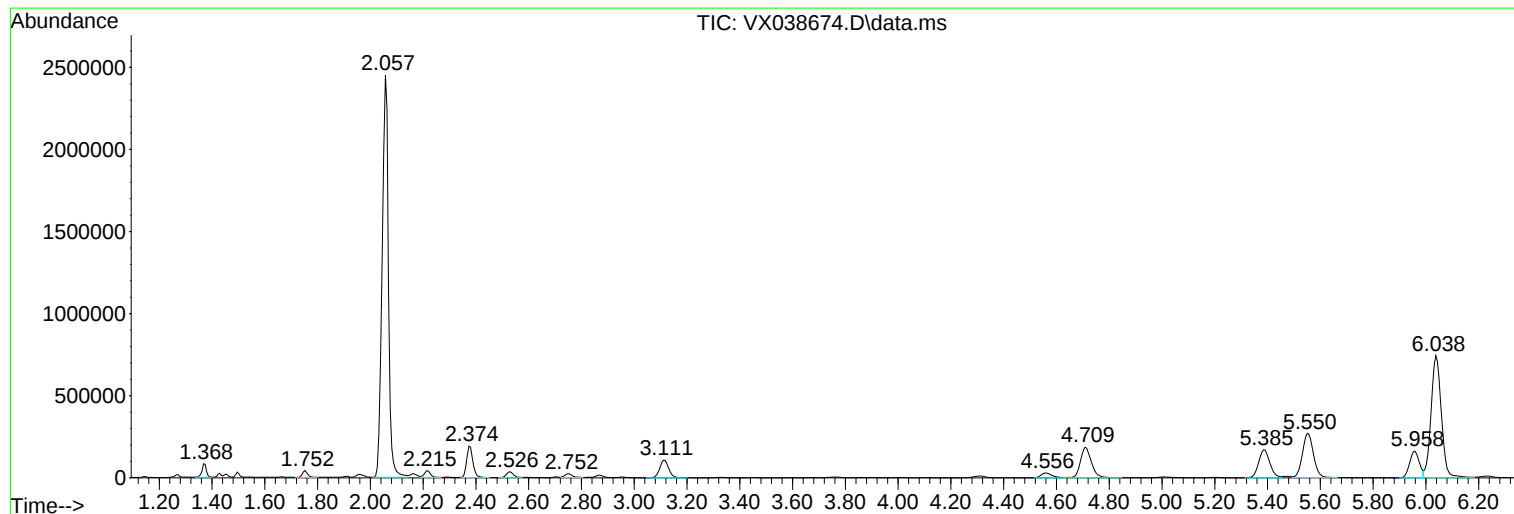
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Quant Title : SW846 8260

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



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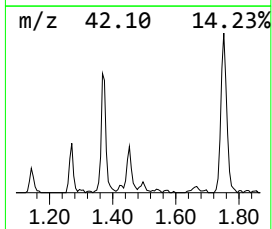
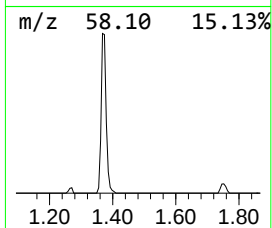
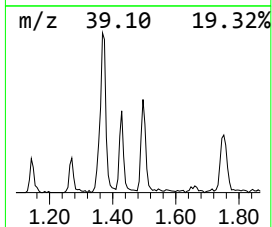
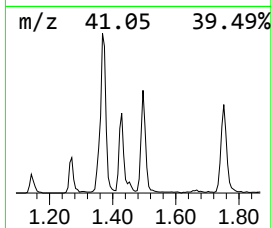
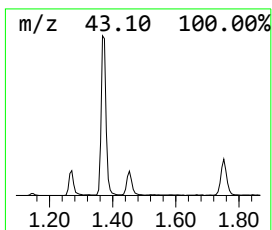
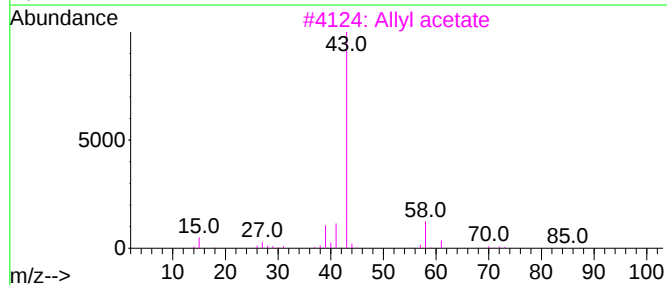
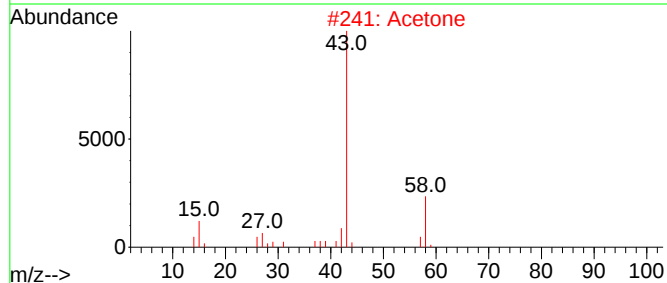
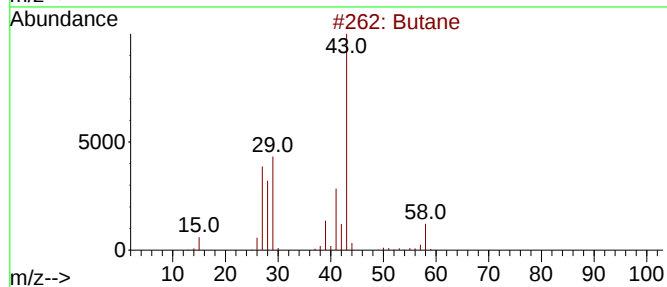
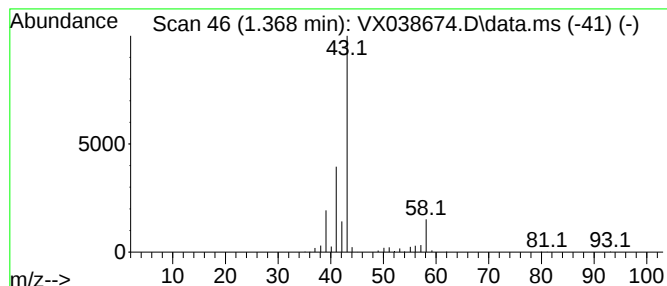
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110723W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.368	6.05 ug/l	94037	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane			58	C4H10	000106-97-8	72
2	Acetone			58	C3H6O	000067-64-1	5
3	Allyl acetate			100	C5H8O2	000591-87-7	4
4	Propane, 2-nitro-			89	C3H7NO2	000079-46-9	4
5	Isobutane			58	C4H10	000075-28-5	4



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Instrument :
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ClientSampleId :
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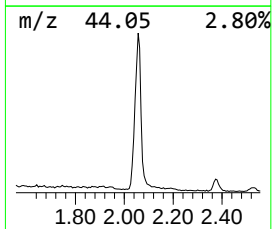
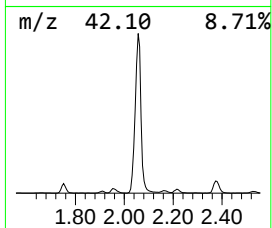
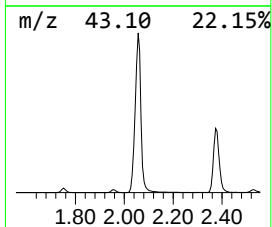
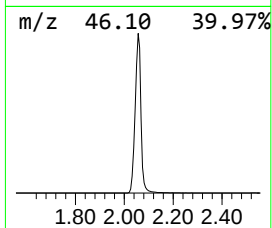
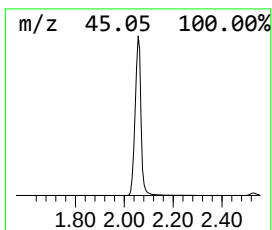
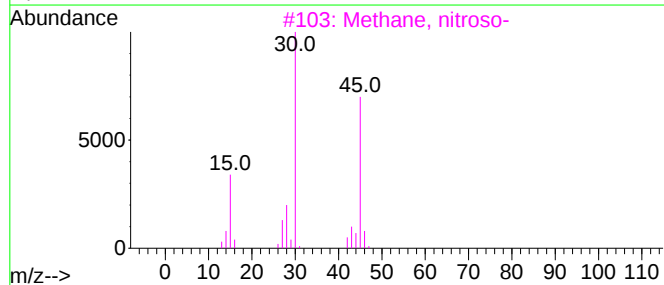
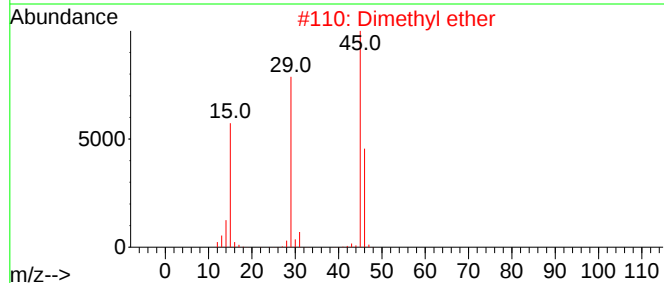
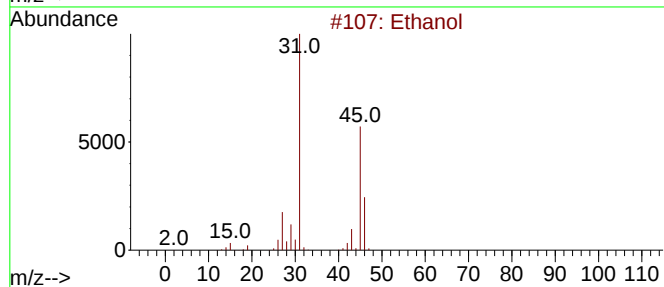
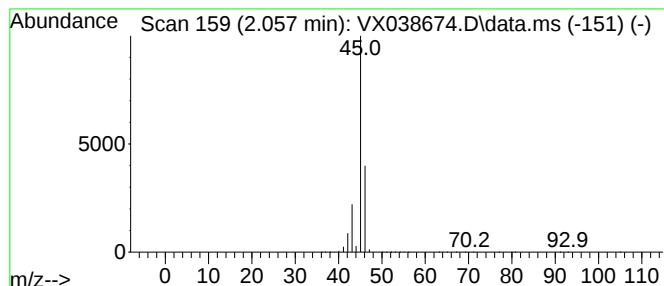
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110723W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.057	259.61 ug/l	4034480	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	78
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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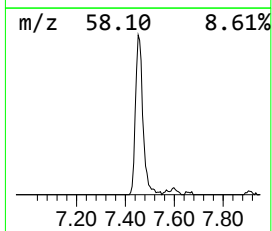
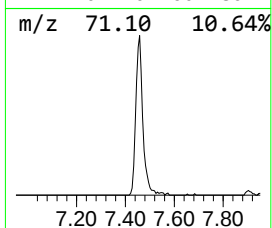
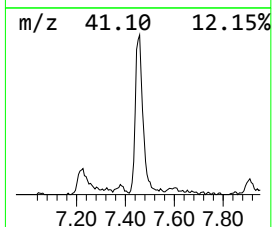
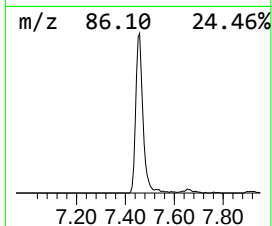
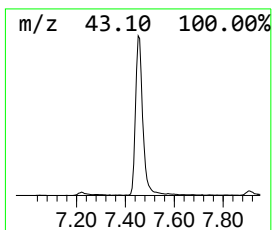
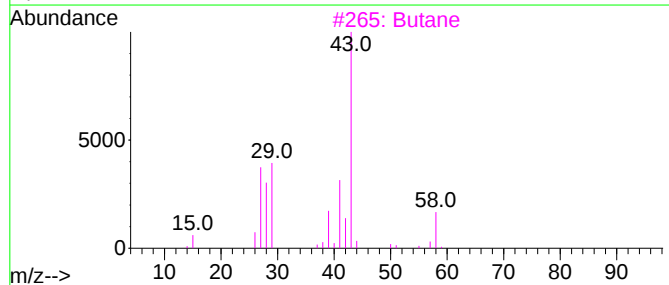
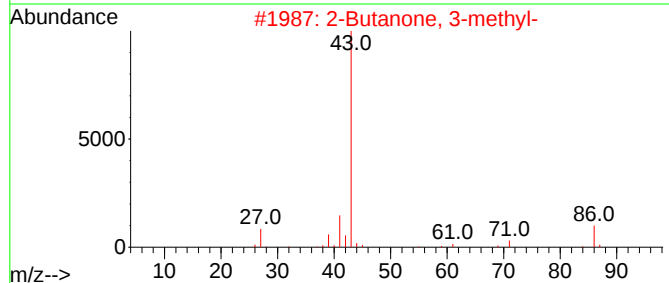
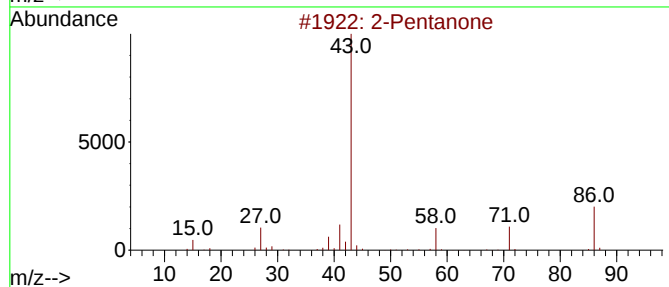
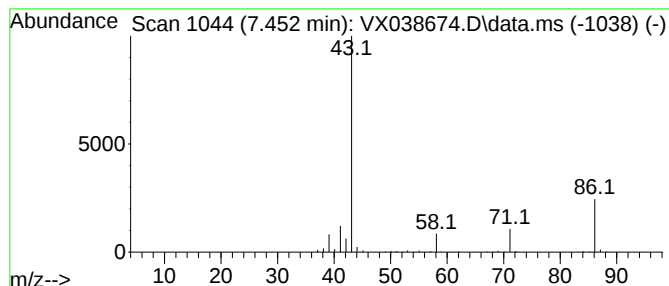
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110723W.M
Quant Title : SW846 8260

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

Peak Number 3 2-Pentanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.452	12.39 ug/l	247349	1,4-Difluorobenzene	6.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone		86	C5H10O	000107-87-9	86
2	2-Butanone, 3-methyl-		86	C5H10O	000563-80-4	59
3	Butane		58	C4H10	000106-97-8	9
4	2,3-Butanedione		86	C4H6O2	000431-03-8	9
5	2-Propanone, methylhydrazone		86	C4H10N2	005771-02-8	9



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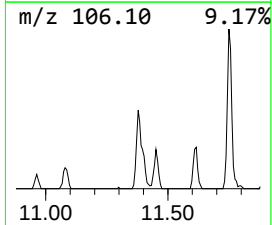
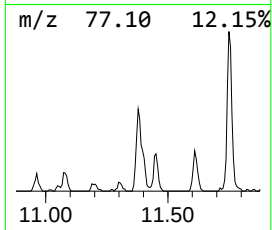
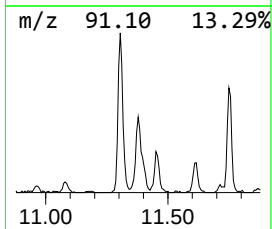
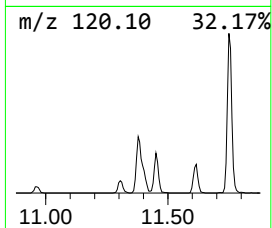
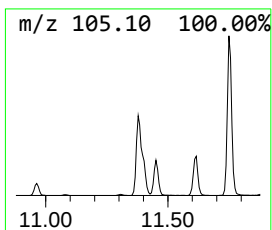
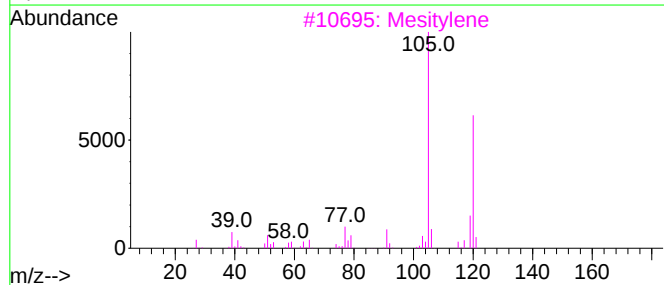
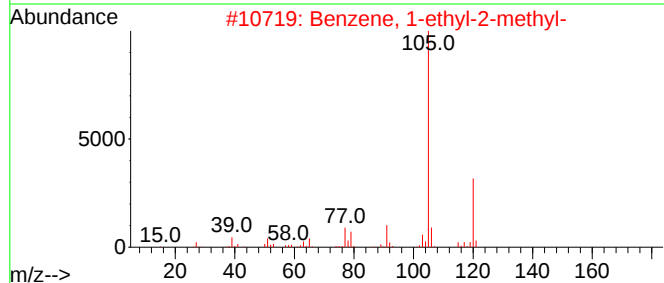
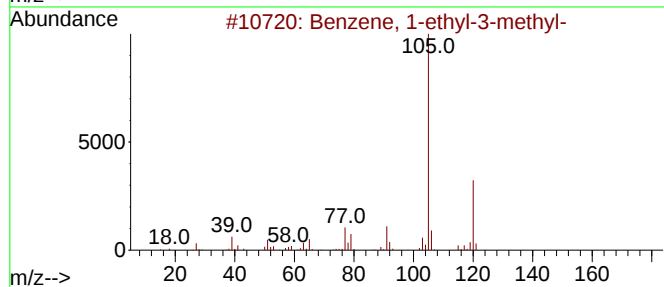
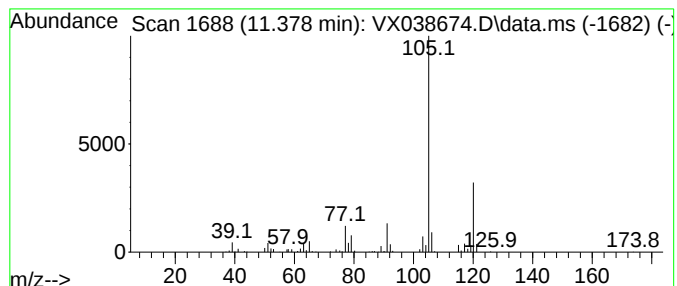
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1-ethyl-3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	5.04 ug/l	153664	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	97
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane	1.368	6.0	ug/l	94037	1	5.550	777017	50.0
Ethanol	2.057	259.6	ug/l	4034480	1	5.550	777017	50.0
2-Pentanone	7.452	12.4	ug/l	247349	2	6.763	998092	50.0
Benzene, 1-ethy...	11.378	5.0	ug/l	153664	4	12.024	1525430	50.0