

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040824\
 Data File : VX040930.D
 Acq On : 08 Apr 2024 15:22
 Operator : JC/MD
 Sample : P2026-02 50X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 50306

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\82X040124W.M
 Title : SW846 8260

Signal : TIC: VX040930.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.270	25	30	36	rBV	3488	3725	1.10%	0.150%
2	1.374	39	47	52	rBV	32834	33056	9.72%	1.335%
3	1.453	58	60	65	rVV	4755	5138	1.51%	0.208%
4	1.495	65	67	71	rVV	3624	3700	1.09%	0.149%
5	1.752	104	109	115	rBV	9211	12266	3.61%	0.495%
6	1.959	138	143	150	rVB3	5352	10754	3.16%	0.434%
7	2.050	152	158	171	rBV	172255	295113	86.80%	11.921%
8	2.166	175	177	181	rVV2	3614	5448	1.60%	0.220%
9	2.215	181	185	192	rVB	9787	15253	4.49%	0.616%
10	2.751	268	273	279	rBV3	3032	5472	1.61%	0.221%
11	2.867	287	292	299	rVB2	2155	4390	1.29%	0.177%
12	3.117	326	333	341	rVB3	3254	7752	2.28%	0.313%
13	3.763	430	439	448	rBB4	1369	3806	1.12%	0.154%
14	4.714	585	595	609	rBV2	21381	62257	18.31%	2.515%
15	5.385	696	705	716	rBV2	26994	80279	23.61%	3.243%
16	5.556	723	733	746	rVB2	41934	118419	34.83%	4.783%
17	5.958	789	799	805	rBV2	32448	85351	25.10%	3.448%
18	6.037	805	812	827	rVB	63549	169875	49.97%	6.862%
19	6.763	922	931	947	rBV	71493	169913	49.98%	6.863%
20	8.647	1234	1240	1246	rBV	150313	235380	69.23%	9.508%
21	8.720	1246	1252	1267	rVB	212947	339984	100.00%	13.733%
22	10.055	1465	1471	1487	rBV	160281	225788	66.41%	9.120%
23	10.195	1489	1494	1500	rBV	16506	22698	6.68%	0.917%
24	10.299	1505	1511	1522	rBB	56746	77351	22.75%	3.124%
25	10.640	1562	1567	1576	rBV	26579	34600	10.18%	1.398%
26	11.079	1634	1639	1652	rVB	145837	182728	53.75%	7.381%
27	11.378	1684	1688	1696	rBV	5739	10198	3.00%	0.412%
28	11.750	1743	1749	1757	rBV	11276	14456	4.25%	0.584%
29	12.018	1788	1793	1801	rBV	182063	236185	69.47%	9.540%
30	12.085	1801	1804	1809	rVB2	3712	4305	1.27%	0.174%

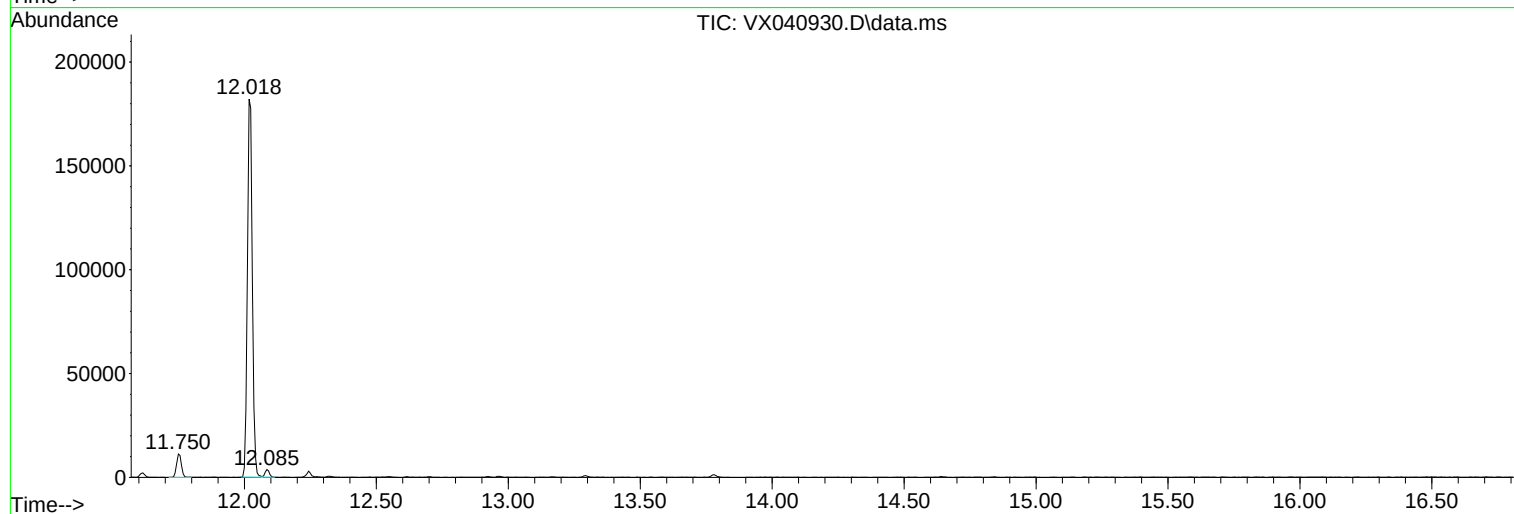
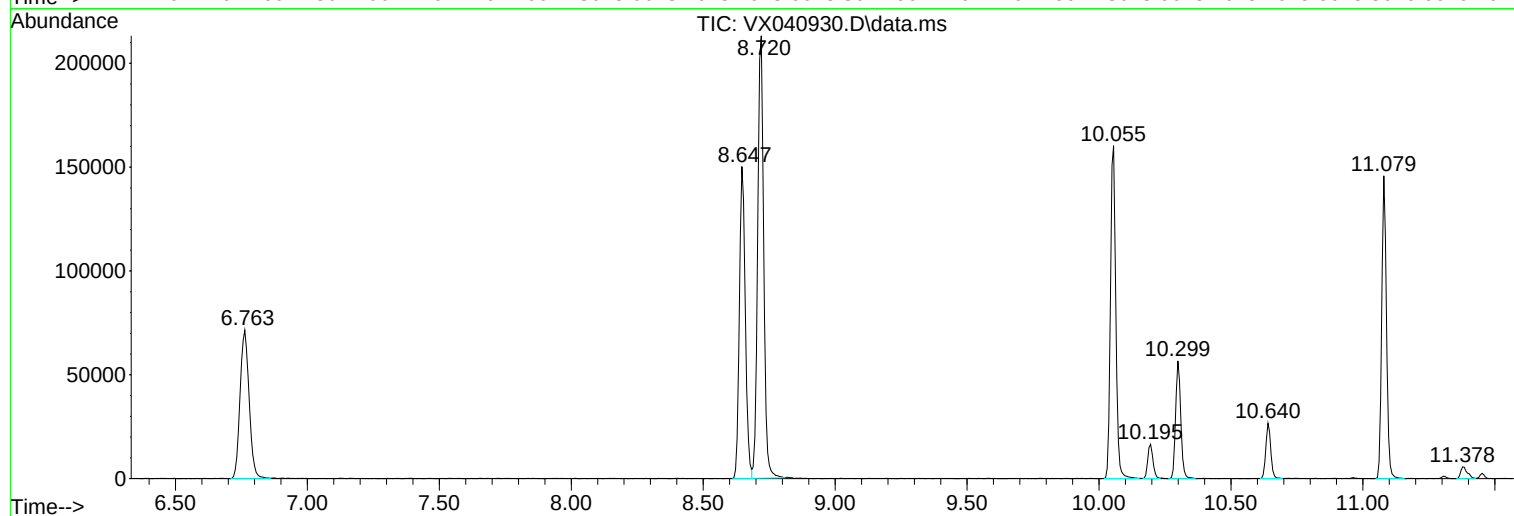
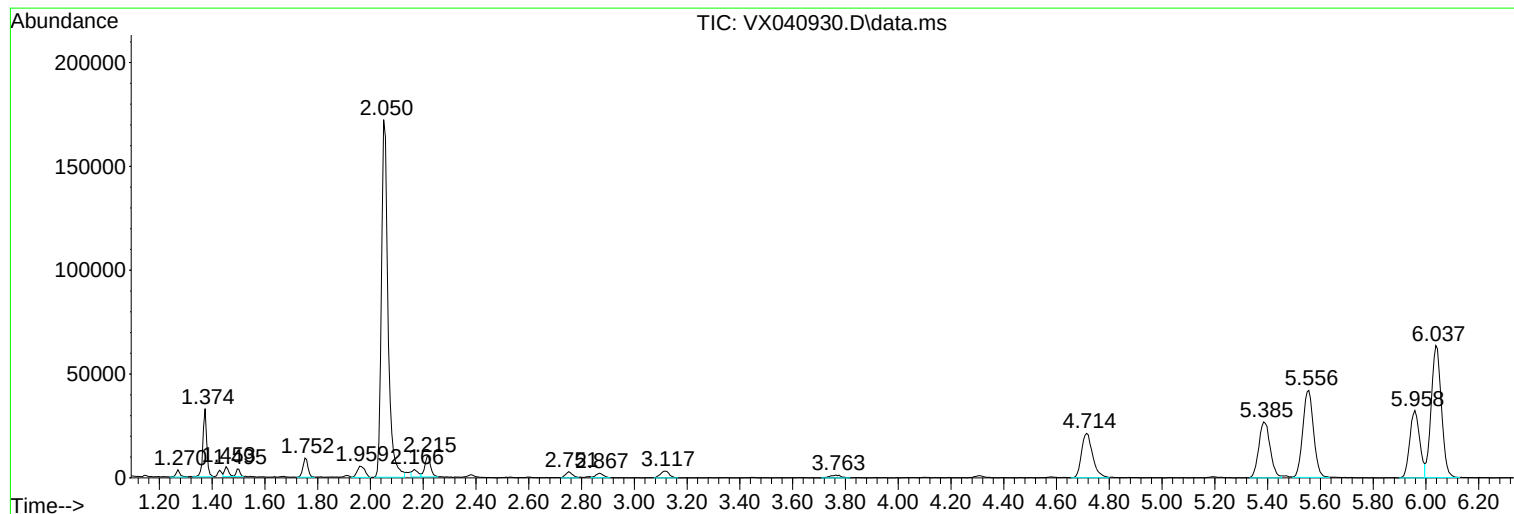
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040124W.M
Quant Title : SW846 8260

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



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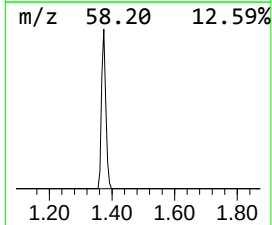
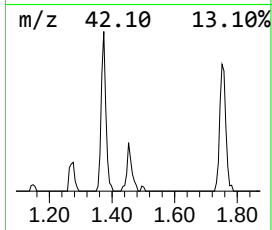
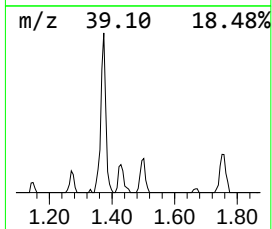
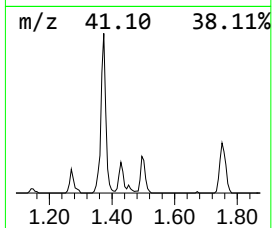
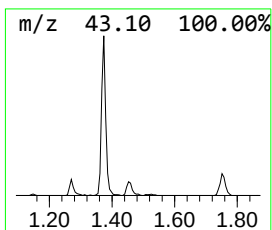
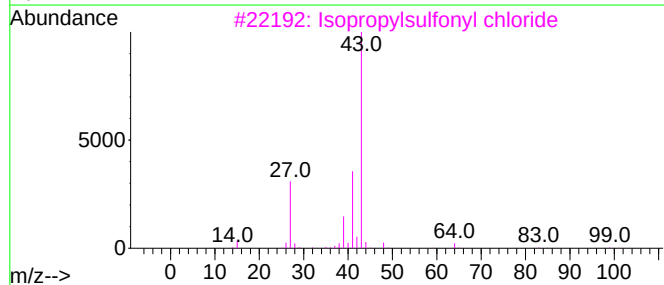
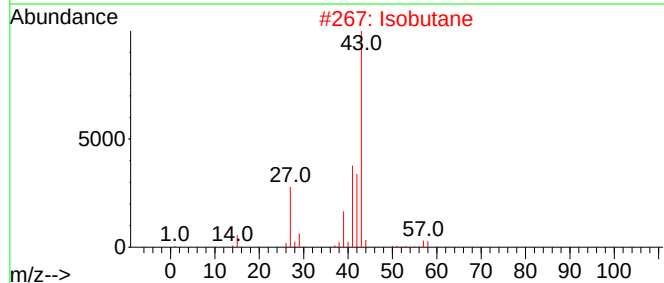
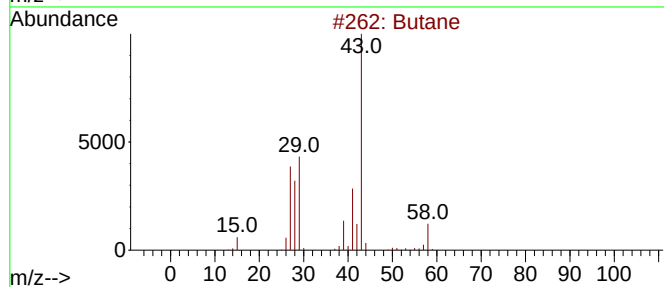
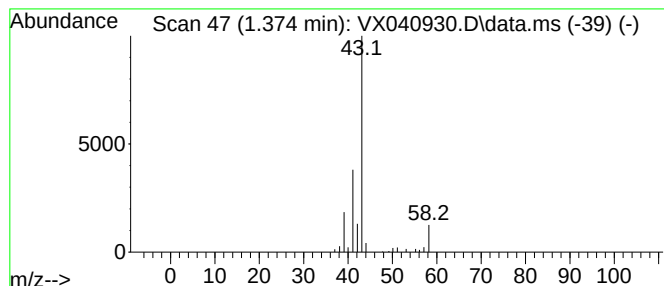
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040124W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.374	13.96 ug/l	33056	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane			58	C4H10	000106-97-8	72
2	Isobutane			58	C4H10	000075-28-5	9
3	Isopropylsulfonyl chloride			142	C3H7ClO2S	010147-37-2	9
4	Propane, 1-nitro-			89	C3H7NO2	000108-03-2	9
5	Diazene, dimethyl-			58	C2H6N2	000503-28-6	4



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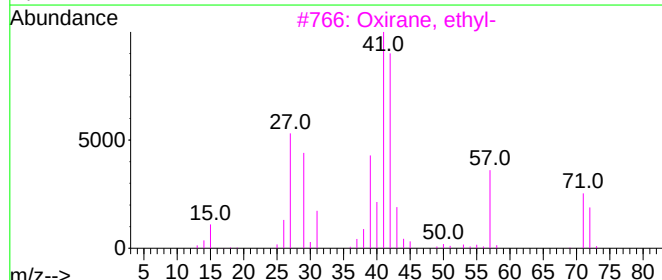
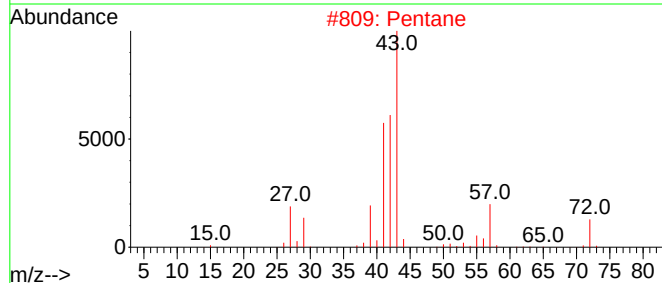
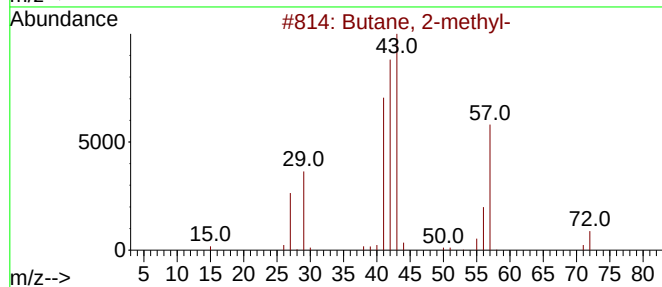
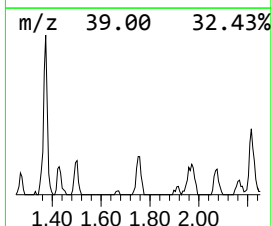
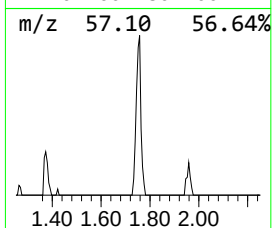
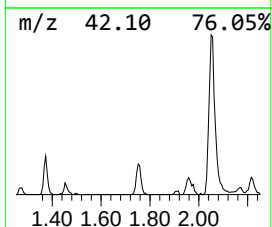
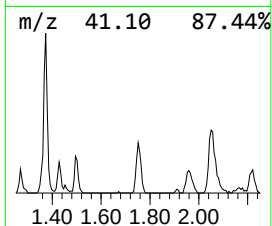
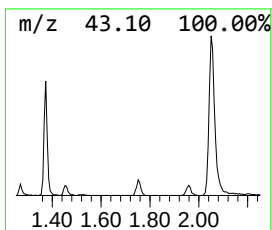
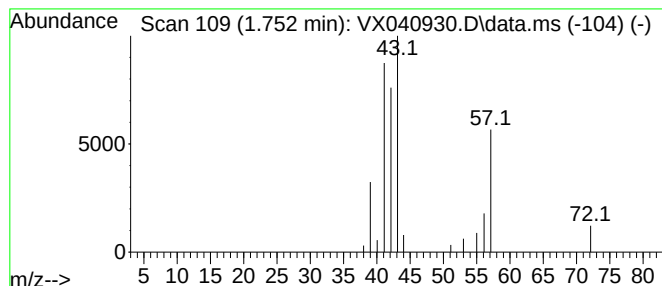
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040124W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	5.18 ug/l	12266	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	90
2			Pentane	72	C5H12	000109-66-0	64
3			Oxirane, ethyl-	72	C4H8O	000106-88-7	42
4			3-Buten-1-ol	72	C4H8O	000627-27-0	40
5			1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	9



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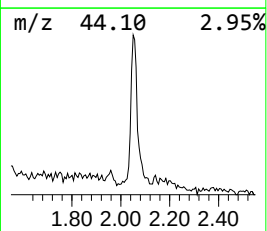
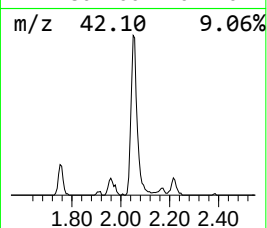
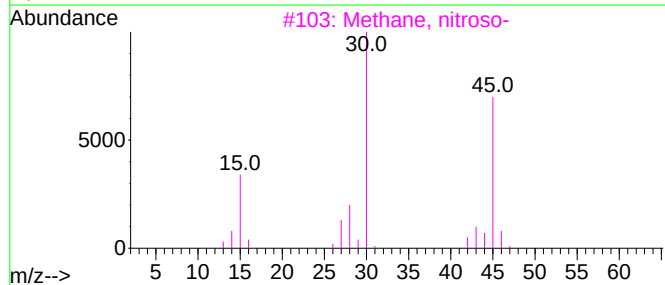
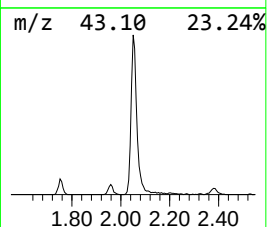
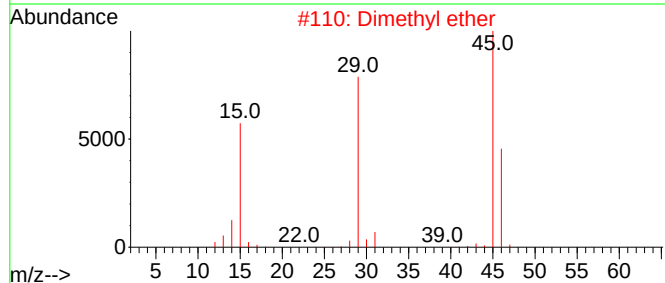
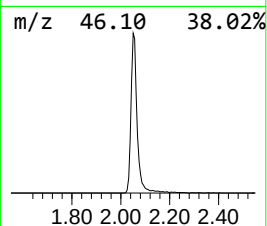
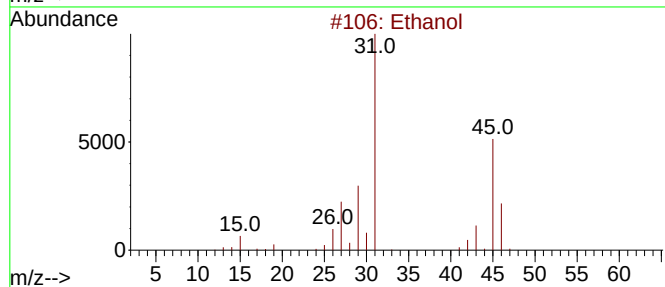
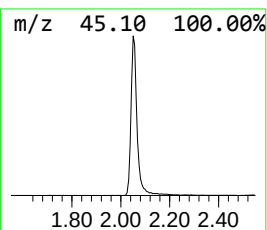
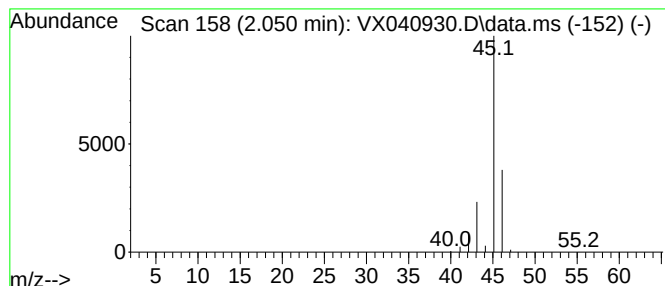
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.050	124.61 ug/l	295113	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	74
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			L-Lactic acid	90	C3H6O3	000079-33-4	2



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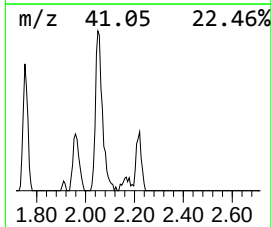
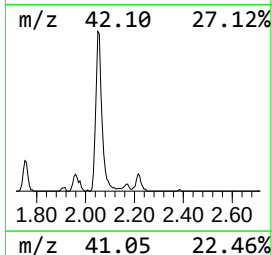
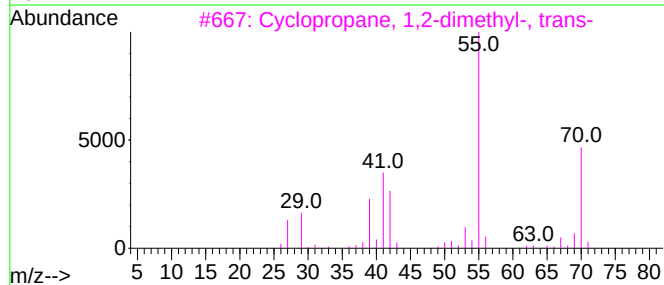
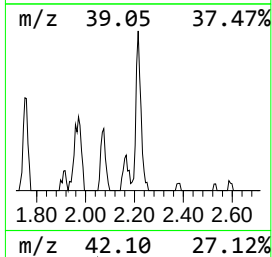
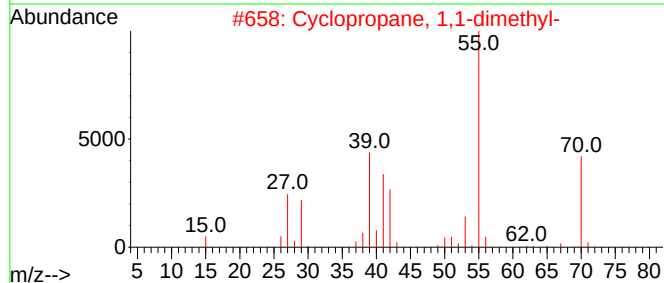
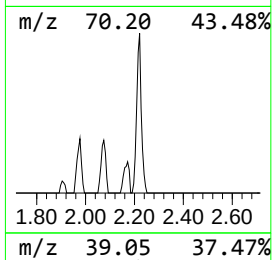
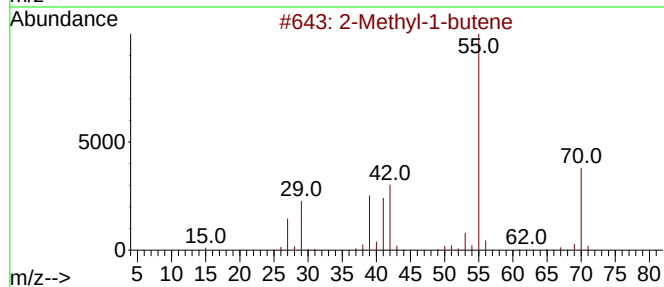
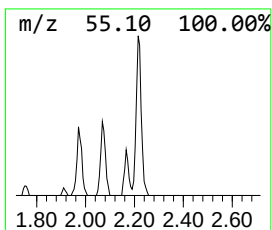
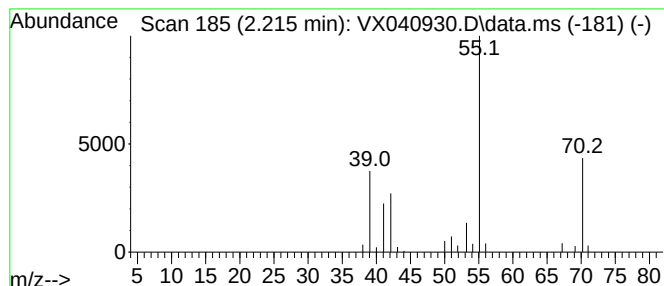
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Peak Number 4 2-Methyl-1-butene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.215	6.44 ug/l	15253	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methyl-1-butene	70	C5H10	000563-46-2	86
2			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80
3			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	80
4			2-Pentene, (Z)-	70	C5H10	000627-20-3	78
5			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	78



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane	1.374	14.0	ug/l	33056	1	5.550	118419	50.0
Butane, 2-methyl-	1.752	5.2	ug/l	12266	1	5.550	118419	50.0
Ethanol	2.050	124.6	ug/l	295113	1	5.550	118419	50.0
2-Methyl-1-butene	2.215	6.4	ug/l	15253	1	5.550	118419	50.0