

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122823\
 Data File : VX039525.D
 Acq On : 28 Dec 2023 18:35
 Operator : JC/MD
 Sample : 06025-02 5X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 50230

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: VX039525.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	21	29	39	rBV3	7084	15413	2.14%	0.262%
2	1.373	41	47	53	rBV	29537	32142	4.47%	0.546%
3	1.453	56	60	65	rVV	130726	154839	21.52%	2.631%
4	1.495	65	67	73	rVB2	13212	19744	2.74%	0.335%
5	1.727	101	105	112	rVB	13991	19773	2.75%	0.336%
6	1.940	136	140	146	rBV2	5298	8777	1.22%	0.149%
7	2.087	155	164	172	rBV	291248	489304	68.02%	8.314%
8	2.209	179	184	193	rVB3	6810	13263	1.84%	0.225%
9	2.385	205	213	225	rVB	28548	48209	6.70%	0.819%
10	2.946	297	305	316	rVB	7911	19939	2.77%	0.339%
11	3.111	324	332	345	rVB	16774	39145	5.44%	0.665%
12	4.300	518	527	540	rVB8	2639	8547	1.19%	0.145%
13	4.574	564	572	573	rBV3	5243	9704	1.35%	0.165%
14	4.720	586	596	617	rVB	41547	122015	16.96%	2.073%
15	5.385	695	705	716	rBV	58525	172137	23.93%	2.925%
16	5.549	722	732	748	rVB	86268	247308	34.38%	4.202%
17	5.952	789	798	805	rBV	70091	185684	25.81%	3.155%
18	6.037	805	812	830	rVB2	141647	389579	54.16%	6.619%
19	6.757	922	930	948	rBV	161209	393966	54.77%	6.694%
20	7.470	1041	1047	1057	rBV	6904	16714	2.32%	0.284%
21	8.646	1234	1240	1246	rBV	352063	549511	76.39%	9.336%
22	8.720	1246	1252	1266	rVB	452594	719365	100.00%	12.222%
23	10.055	1465	1471	1485	rBV	378355	524117	72.86%	8.905%
24	10.195	1489	1494	1505	rVB	39324	53706	7.47%	0.912%
25	10.299	1505	1511	1523	rBV	113243	162613	22.61%	2.763%
26	10.640	1562	1567	1578	rVB	61726	86135	11.97%	1.463%
27	11.079	1634	1639	1652	rBV	301194	395785	55.02%	6.725%
28	11.378	1684	1688	1697	rVV	20622	37991	5.28%	0.645%
29	11.451	1697	1700	1707	rVB	10169	12833	1.78%	0.218%
30	11.615	1720	1727	1734	rBV	10536	14140	1.97%	0.240%
31	11.750	1745	1749	1762	rVB	43812	58502	8.13%	0.994%
32	12.024	1788	1794	1800	rBV	352962	470504	65.41%	7.994%
33	12.085	1800	1804	1812	rVB	18668	25927	3.60%	0.441%
34	12.243	1823	1830	1833	rBV2	16003	22533	3.13%	0.383%
35	12.316	1838	1842	1851	rVB2	9804	14202	1.97%	0.241%
36	12.615	1886	1891	1894	rBV	7972	9744	1.35%	0.166%

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37	12.701	1900	1905	1915	rBV2	7142	12507	1.74%	0.213%
38	12.920	1934	1941	1944	rBV	6421	8588	1.19%	0.146%
39	12.963	1944	1948	1953	rVB	10039	12859	1.79%	0.218%
40	13.170	1973	1982	1986	rBV	11816	16785	2.33%	0.285%
41	13.292	1998	2002	2007	rVB2	25786	33927	4.72%	0.576%
42	13.420	2019	2023	2032	rVB	21948	27706	3.85%	0.471%
43	13.585	2046	2050	2056	rVV4	6678	11749	1.63%	0.200%
44	13.664	2056	2063	2070	rVB3	6779	15471	2.15%	0.263%
45	13.780	2074	2082	2089	rBV2	12012	18885	2.63%	0.321%
46	13.853	2089	2094	2099	rVB	9925	12985	1.81%	0.221%
47	13.926	2099	2106	2110	rBV2	10615	15214	2.11%	0.258%
48	14.072	2127	2130	2135	rVB	7672	9237	1.28%	0.157%
49	14.231	2148	2156	2161	rBV3	25413	41303	5.74%	0.702%
50	14.371	2175	2179	2183	rVV2	8750	10454	1.45%	0.178%
51	14.481	2192	2197	2203	rBV3	17651	24036	3.34%	0.408%
52	14.615	2215	2219	2220	rBV2	8983	10131	1.41%	0.172%
53	14.639	2220	2223	2226	rVV2	10922	16159	2.25%	0.275%
54	14.670	2226	2228	2233	rVB3	5919	7301	1.01%	0.124%
55	15.182	2307	2312	2320	rBV2	9292	16519	2.30%	0.281%

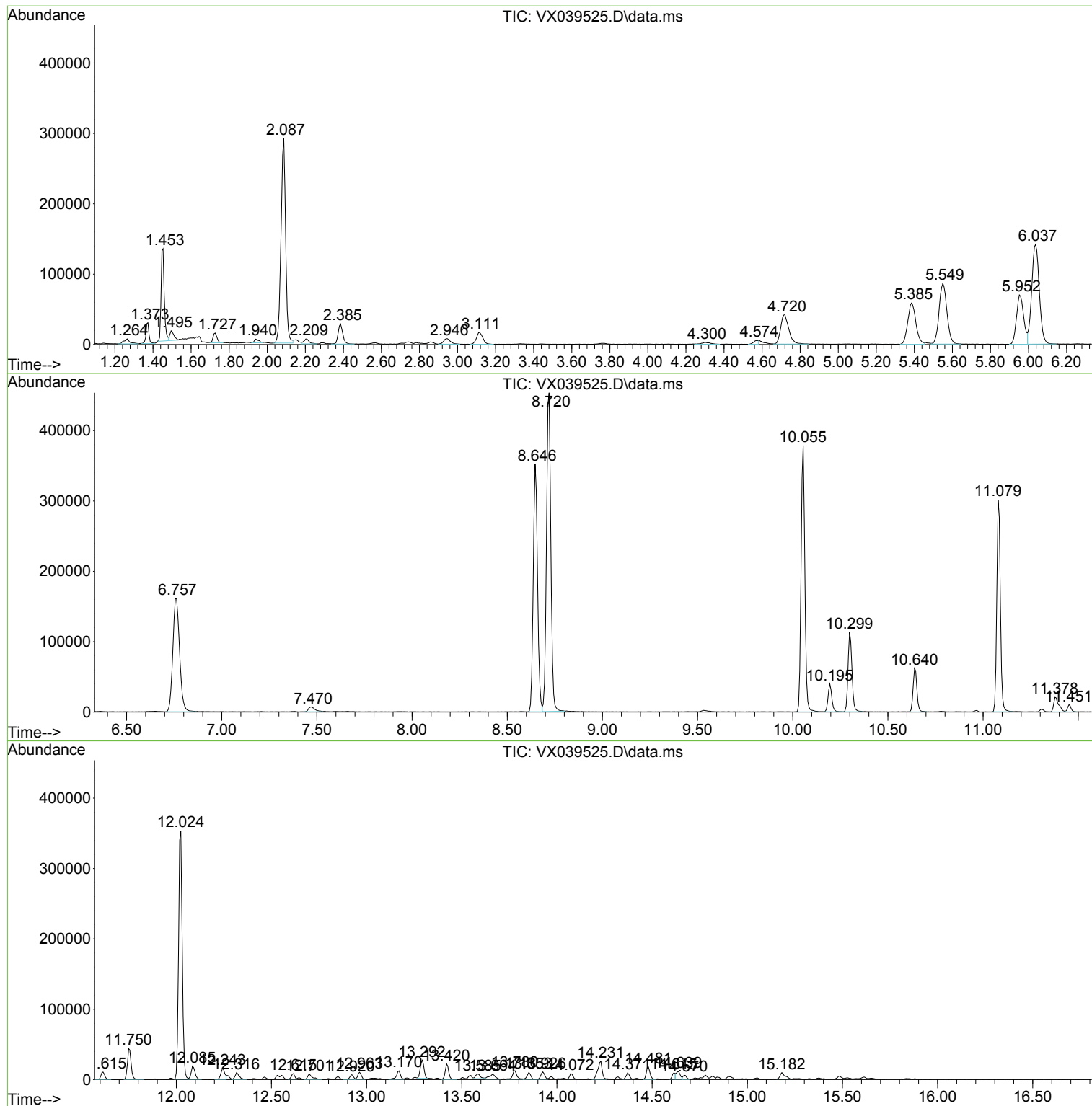
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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



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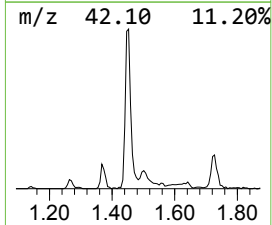
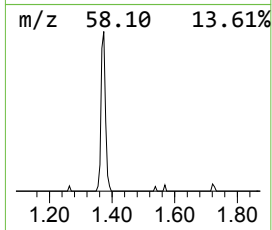
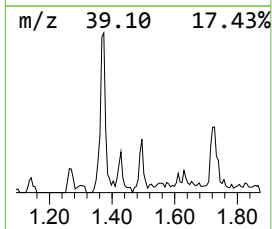
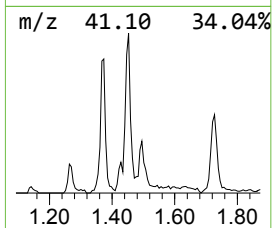
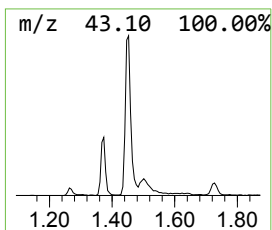
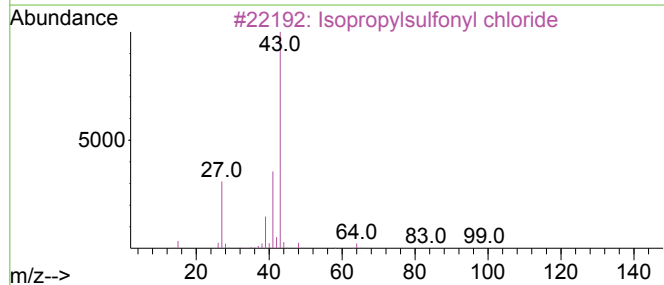
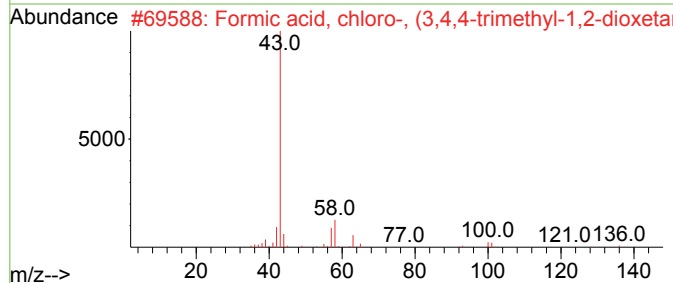
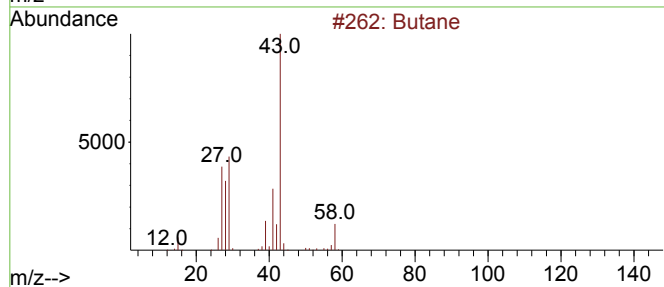
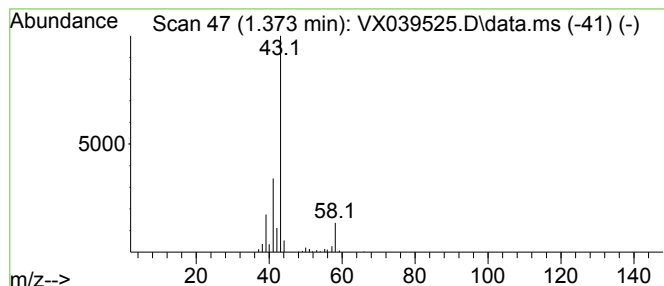
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.373	6.50 ug/l	32142	Pentafluorobenzene	5.549

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	72
2			Formic acid, chloro-, (3,4,4-tri...	194	C7H11ClO4	107323-92-2	40
3			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
4			Isobutane	58	C4H10	000075-28-5	9
5			Propane, 2-nitro-	89	C3H7NO2	000079-46-9	9



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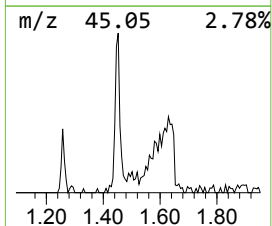
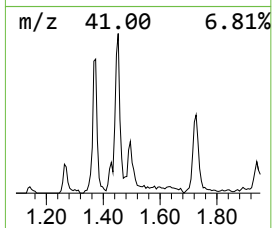
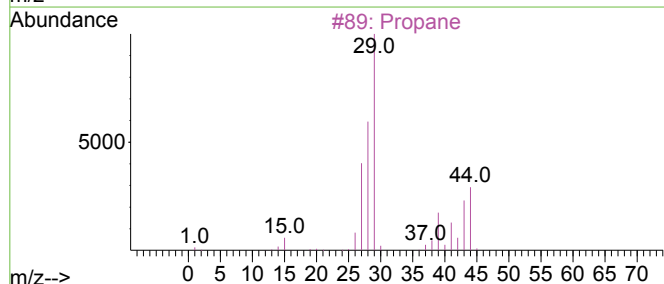
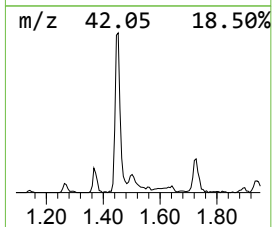
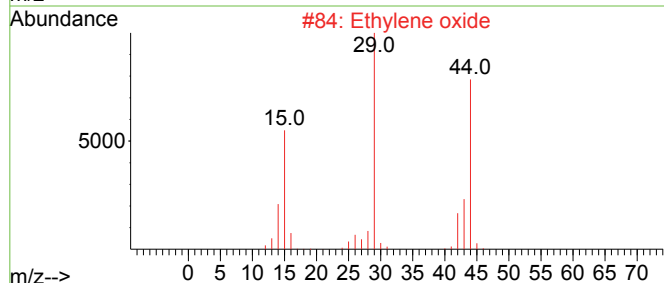
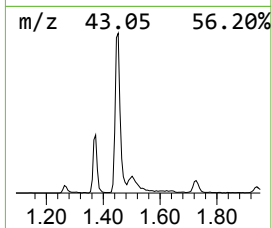
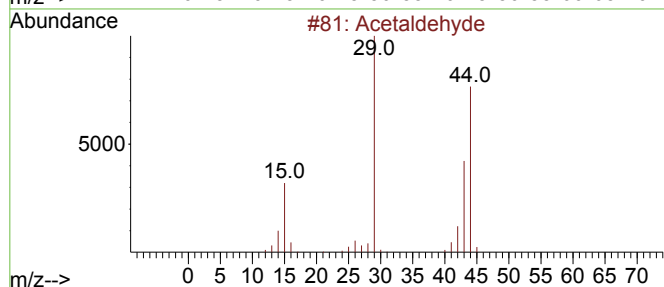
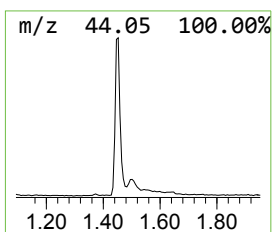
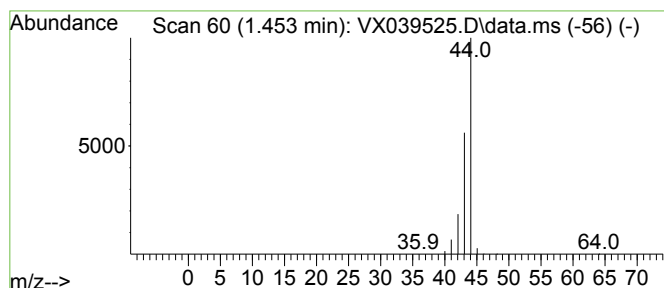
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

Peak Number 2 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.453	31.30 ug/l	154839	Pentafluorobenzene	5.549

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	74
2			Ethylene oxide	44	C2H4O	000075-21-8	5
3			Propane	44	C3H8	000074-98-6	4
4			1,2-Propanediamine	74	C3H10N2	000078-90-0	4
5			Alanine	89	C3H7NO2	000056-41-7	4



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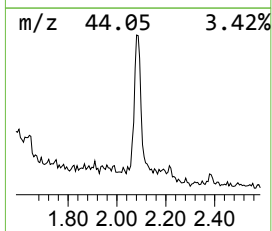
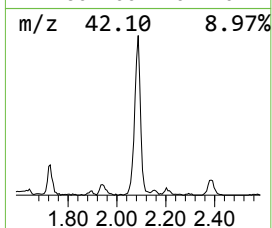
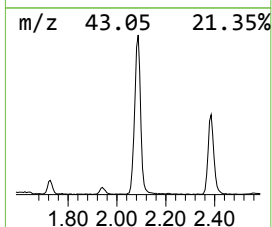
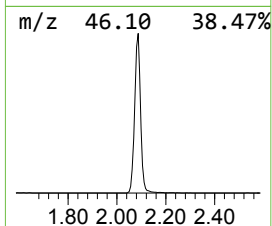
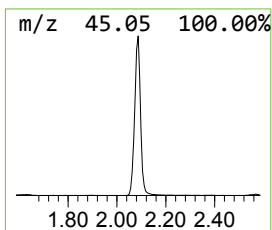
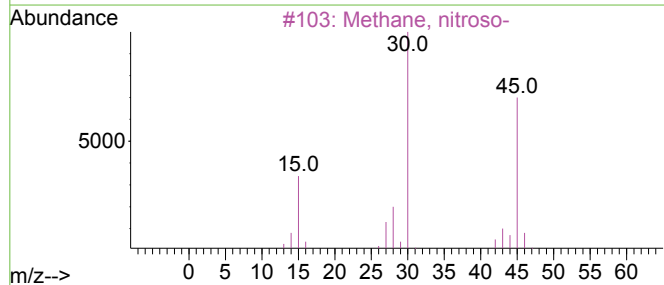
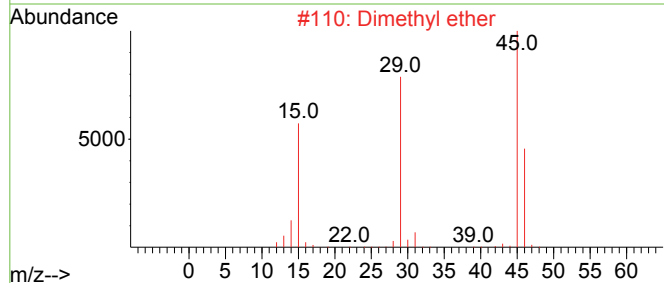
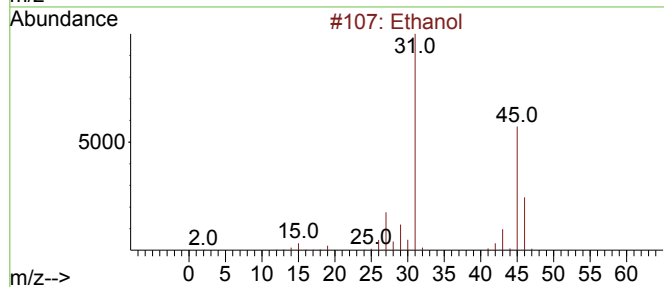
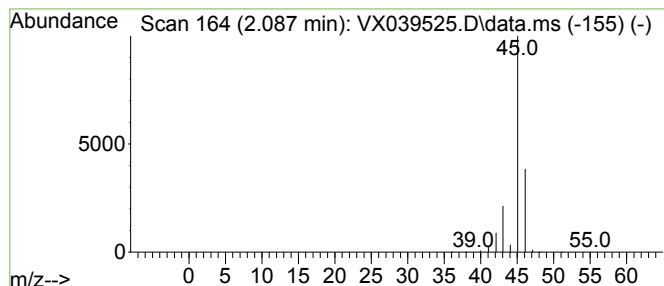
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Quant Title : SW846 8260

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

Peak Number 3 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.087	98.93 ug/l	489304	Pentafluorobenzene	5.549

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	L-Lactic acid			90	C3H6O3	000079-33-4	2



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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	1.373	6.5	ug/l	32142	1	5.549	247308	50.0
Acetaldehyde	1.453	31.3	ug/l	154839	1	5.549	247308	50.0
Ethanol	2.087	98.9	ug/l	489304	1	5.549	247308	50.0