

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122823\
 Data File : VX039524.D
 Acq On : 28 Dec 2023 18:12
 Operator : JC/MD
 Sample : 06025-01 5X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 50200

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: VX039524.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	26	29	37	rVB2	13609	16827	2.41%	0.317%
2	1.368	41	46	52	rBV	81049	86038	12.31%	1.621%
3	1.429	52	56	57	rBV	8294	9281	1.33%	0.175%
4	1.447	57	59	64	rVB	38269	41066	5.87%	0.774%
5	1.496	64	67	72	rVB2	11469	12469	1.78%	0.235%
6	1.624	72	88	89	rBV9	6101	22871	3.27%	0.431%
7	1.721	99	104	111	rBV	31467	44097	6.31%	0.831%
8	1.941	136	140	148	rVB2	11049	19675	2.81%	0.371%
9	2.087	154	164	171	rBV	176873	305441	43.69%	5.756%
10	2.154	171	175	179	rVV2	7047	12375	1.77%	0.233%
11	2.203	179	183	193	rVB	15168	26150	3.74%	0.493%
12	2.386	207	213	221	rVB	23240	39544	5.66%	0.745%
13	2.739	261	271	275	rBV3	5368	12216	1.75%	0.230%
14	2.861	286	291	297	rVB2	5254	9896	1.42%	0.186%
15	2.947	297	305	312	rVB	5386	12631	1.81%	0.238%
16	3.117	324	333	341	rBV2	12223	30527	4.37%	0.575%
17	4.294	517	526	537	rVB4	3553	10918	1.56%	0.206%
18	4.581	566	573	578	rBV2	2811	7814	1.12%	0.147%
19	4.721	588	596	614	rVB2	15539	46035	6.59%	0.867%
20	5.385	694	705	718	rBV2	64522	192057	27.47%	3.619%
21	5.550	722	732	746	rVB	96363	273850	39.18%	5.160%
22	5.952	788	798	805	rBV	78170	208244	29.79%	3.924%
23	6.038	805	812	830	rVB	137451	372715	53.32%	7.023%
24	6.757	921	930	947	rBV	177279	433111	61.96%	8.161%
25	7.476	1040	1048	1056	rBV2	3928	9947	1.42%	0.187%
26	8.647	1232	1240	1246	rBV	381216	593109	84.85%	11.176%
27	8.714	1246	1251	1270	rVB	439884	699039	100.00%	13.172%
28	10.055	1465	1471	1489	rBV	384169	540188	77.28%	10.179%
29	10.195	1489	1494	1503	rVB	35800	49294	7.05%	0.929%
30	10.299	1505	1511	1523	rBV	110593	153830	22.01%	2.899%
31	10.640	1562	1567	1574	rBV	58669	76007	10.87%	1.432%
32	11.079	1634	1639	1655	rBV	307634	397164	56.82%	7.484%
33	11.378	1684	1688	1697	rBV	10506	19607	2.80%	0.369%
34	11.750	1745	1749	1757	rBV	22502	28450	4.07%	0.536%
35	12.024	1788	1794	1801	rBV	339112	451796	64.63%	8.513%
36	12.085	1801	1804	1812	rVB	9771	12895	1.84%	0.243%

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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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37	12.244	1821	1830	1839	rBV3	7149	10850	1.55%	0.204%
38	13.292	1997	2002	2006	rBV3	5869	7677	1.10%	0.145%
39	13.780	2075	2082	2091	rVB	8293	11134	1.59%	0.210%

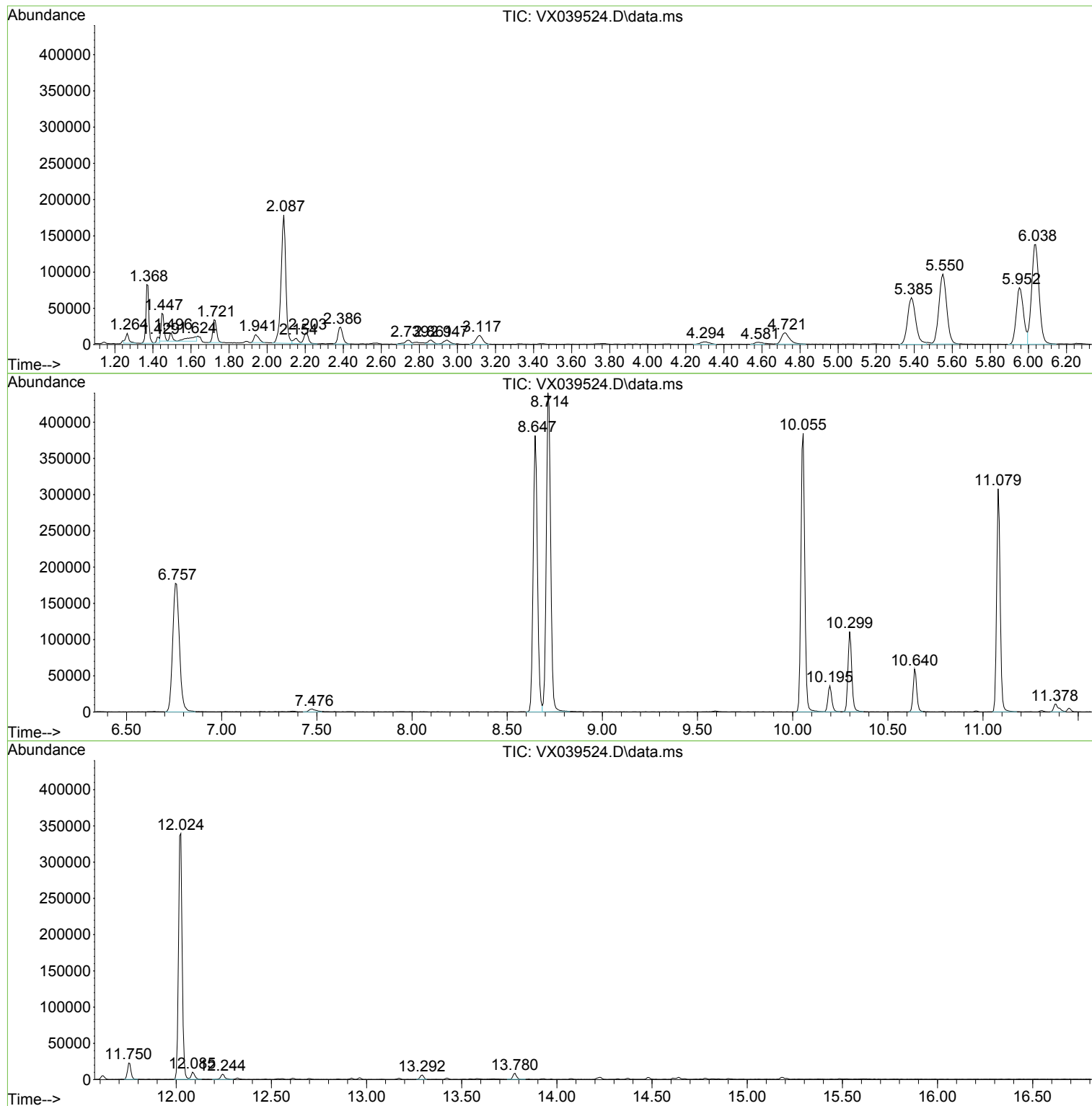
Sum of corrected areas: 5306835

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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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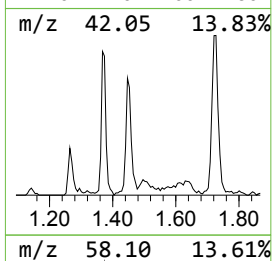
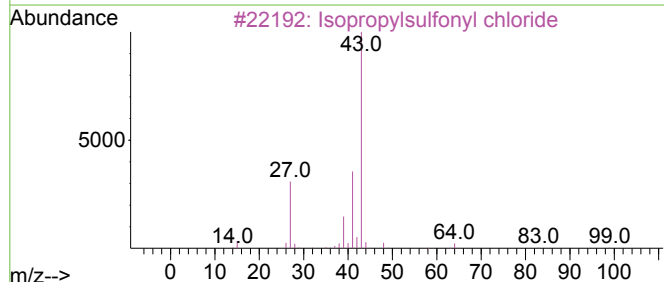
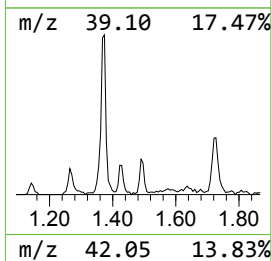
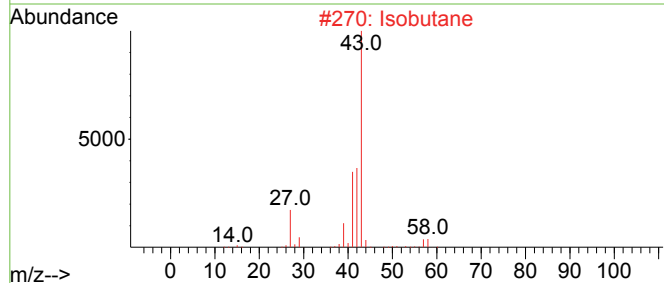
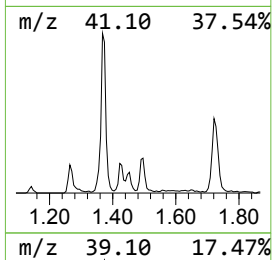
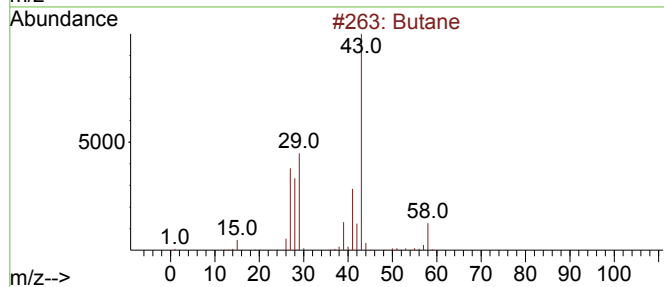
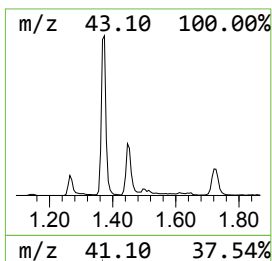
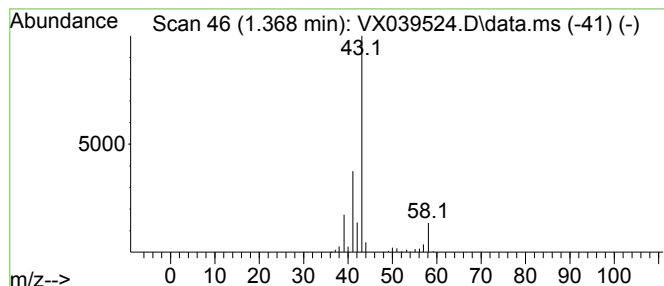
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
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Peak Number 1 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.368	15.71 ug/l	86038	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	80
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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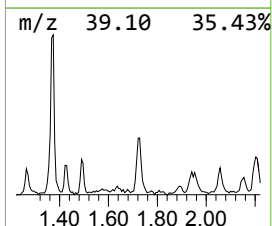
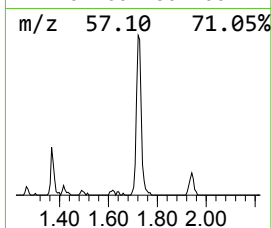
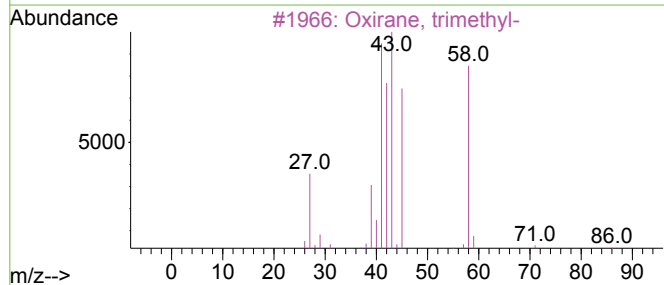
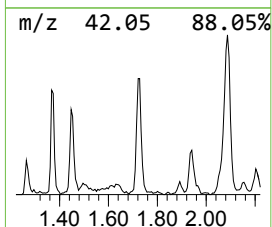
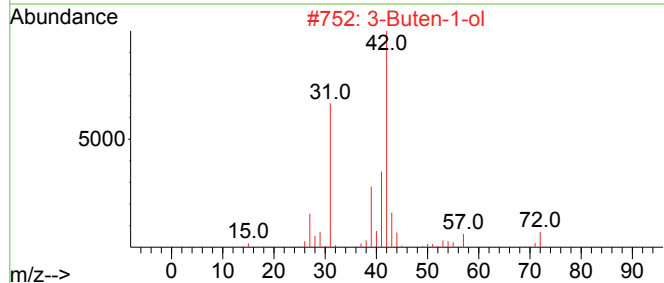
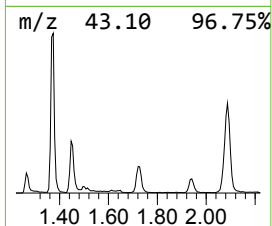
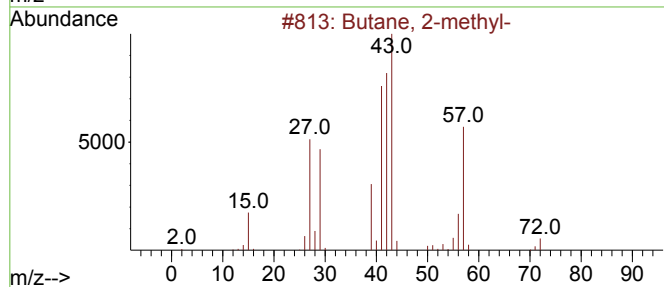
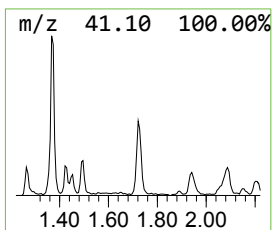
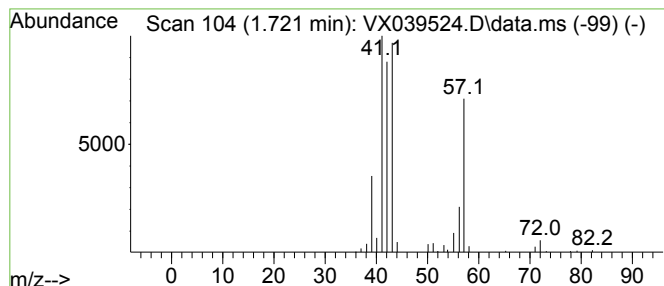
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.721	8.05 ug/l	44097	Pentafluorobenzene	5.550

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methyl-	72	C5H12	000078-78-4	87
2		3-Buten-1-ol	72	C4H8O	000627-27-0	47
3		Oxirane, trimethyl-	86	C5H10O	005076-19-7	42
4		Isobutylene epoxide	72	C4H8O	000558-30-5	40
5		Pentane	72	C5H12	000109-66-0	33



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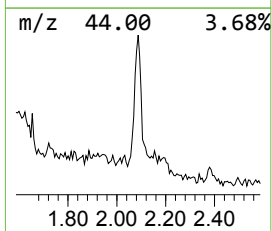
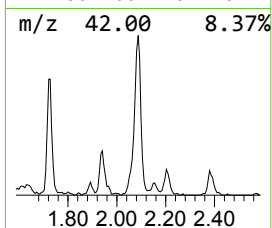
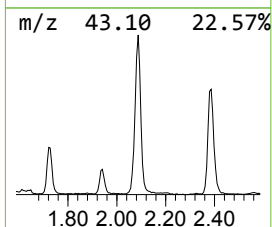
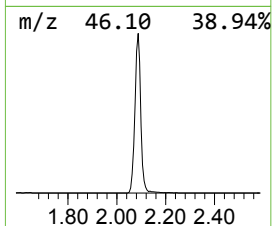
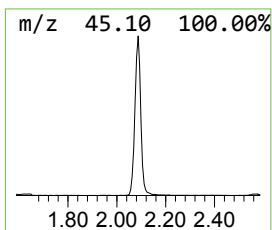
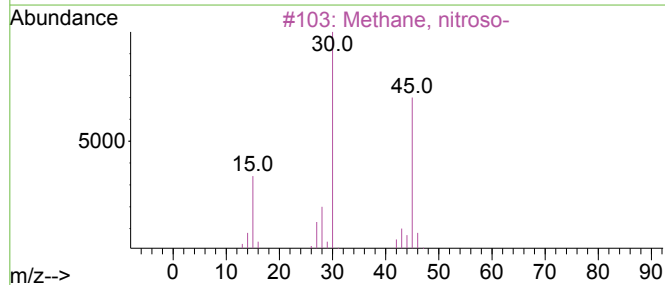
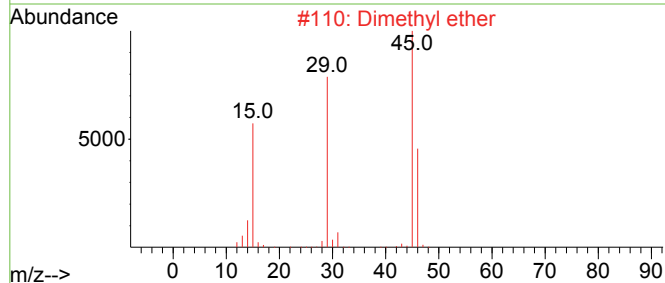
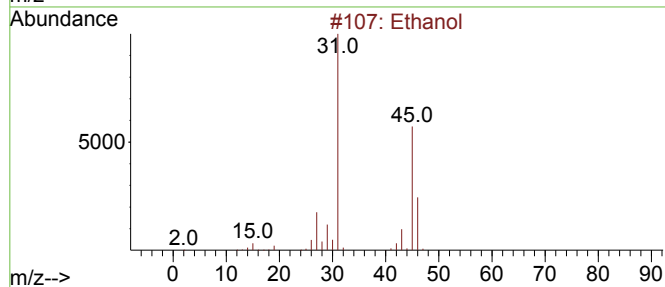
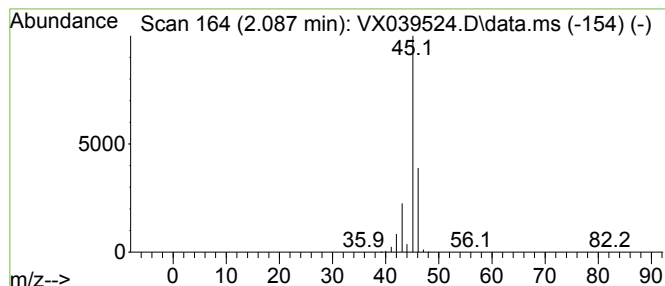
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Quant Title : SW846 8260

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

Peak Number 4 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.087	55.77 ug/l	305441	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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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
Butane	1.368	15.7	ug/l	86038	1	5.550	273850	50.0
Butane, 2-methyl-	1.721	8.1	ug/l	44097	1	5.550	273850	50.0
Ethanol	2.087	55.8	ug/l	305441	1	5.550	273850	50.0