

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052421\
 Data File : VX022158.D
 Acq On : 24 May 2021 19:21
 Operator : JC/MD
 Sample : M2504-04
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-104

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\82X051921W.M
 Title : SW846 8260

Signal : TIC: VX022158.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	28	rBV	14639	17443	3.65%	0.572%
2	1.270	28	30	34	rVB	11090	11166	2.33%	0.366%
3	1.368	43	46	52	rVB	51098	51809	10.83%	1.700%
4	1.550	72	76	81	rBV7	2785	5297	1.11%	0.174%
5	1.752	104	109	116	rBV	36603	50656	10.59%	1.662%
6	1.953	138	142	151	rVB2	16352	26950	5.63%	0.884%
7	2.069	156	161	169	rVV	12649	18384	3.84%	0.603%
8	2.160	172	176	180	rVV2	5038	8093	1.69%	0.266%
9	2.215	182	185	190	rVB	8155	11434	2.39%	0.375%
10	2.550	235	240	248	rBV	3620	6241	1.30%	0.205%
11	2.782	271	278	282	rBV	7545	15021	3.14%	0.493%
12	2.867	290	292	301	rVB5	3159	5642	1.18%	0.185%
13	3.111	322	332	340	rBV3	4522	11346	2.37%	0.372%
14	3.446	382	387	393	rBV5	2071	5162	1.08%	0.169%
15	4.221	505	514	520	rBV5	2139	6854	1.43%	0.225%
16	4.306	522	528	536	rVB3	4752	11847	2.48%	0.389%
17	5.397	694	707	717	rBV2	52953	147919	30.93%	4.854%
18	5.562	722	734	755	rVB2	79869	239278	50.03%	7.853%
19	5.964	790	800	811	rBV	59780	161961	33.86%	5.315%
20	6.257	838	848	858	rVB3	7604	23835	4.98%	0.782%
21	6.769	923	932	943	rBV	145062	342026	71.51%	11.224%
22	7.385	1021	1033	1039	rVB8	1793	5067	1.06%	0.166%
23	7.988	1125	1132	1137	rBV4	3455	7157	1.50%	0.235%
24	8.110	1144	1152	1162	rBV5	4236	9744	2.04%	0.320%
25	8.653	1234	1241	1250	rBV	319415	478276	100.00%	15.696%
26	9.275	1339	1343	1348	rVB3	4222	6005	1.26%	0.197%
27	10.055	1466	1471	1478	rBV	293382	393651	82.31%	12.919%
28	10.195	1489	1494	1504	rVB	36440	48214	10.08%	1.582%
29	10.305	1507	1512	1521	rBV	58697	77766	16.26%	2.552%
30	11.085	1634	1640	1650	rBV	227691	285278	59.65%	9.362%
31	11.305	1672	1676	1680	rBV	5105	5979	1.25%	0.196%
32	11.384	1683	1689	1690	rBV2	12781	14653	3.06%	0.481%
33	11.402	1690	1692	1696	rVV	12165	13615	2.85%	0.447%
34	11.457	1696	1701	1710	rVB	14915	19549	4.09%	0.642%
35	11.616	1719	1727	1732	rBV	8599	10850	2.27%	0.356%
36	11.756	1745	1750	1755	rVB	50060	60797	12.71%	1.995%

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37	12.024	1789	1794	1800	rBV	285212	343863	71.90%	11.285%
38	12.091	1800	1805	1811	rVB	8358	9905	2.07%	0.325%
39	12.250	1825	1831	1838	rBV4	10077	15382	3.22%	0.505%
40	12.317	1838	1842	1848	rVB4	5256	7541	1.58%	0.247%
41	12.616	1886	1891	1894	rBV	4234	4986	1.04%	0.164%
42	12.701	1902	1905	1910	rVB2	7013	8459	1.77%	0.278%
43	13.298	1998	2003	2008	rVB3	6909	8867	1.85%	0.291%
44	13.780	2076	2082	2087	rBV	17370	21730	4.54%	0.713%
45	14.640	2217	2223	2228	rBV	8938	11457	2.40%	0.376%

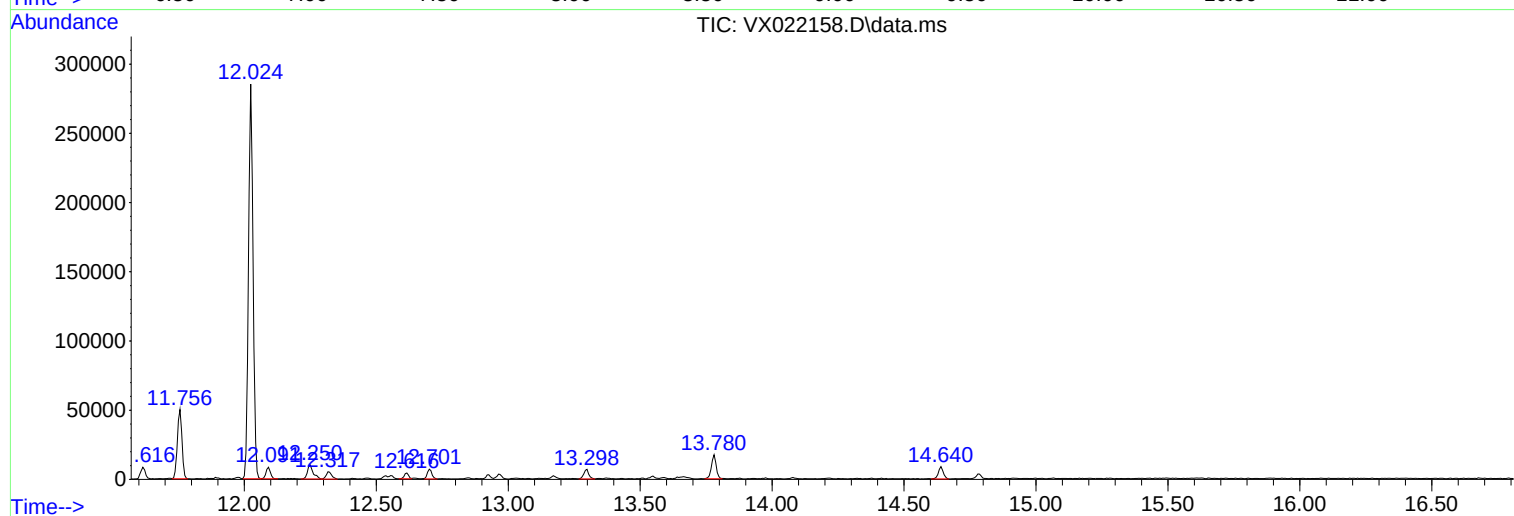
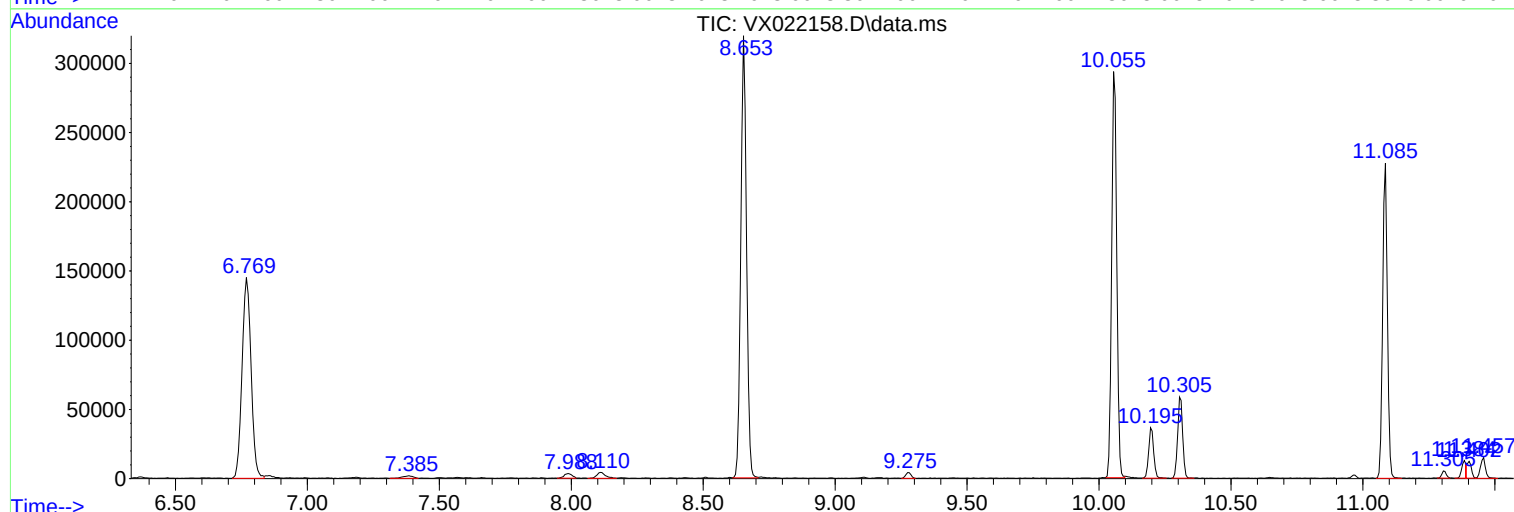
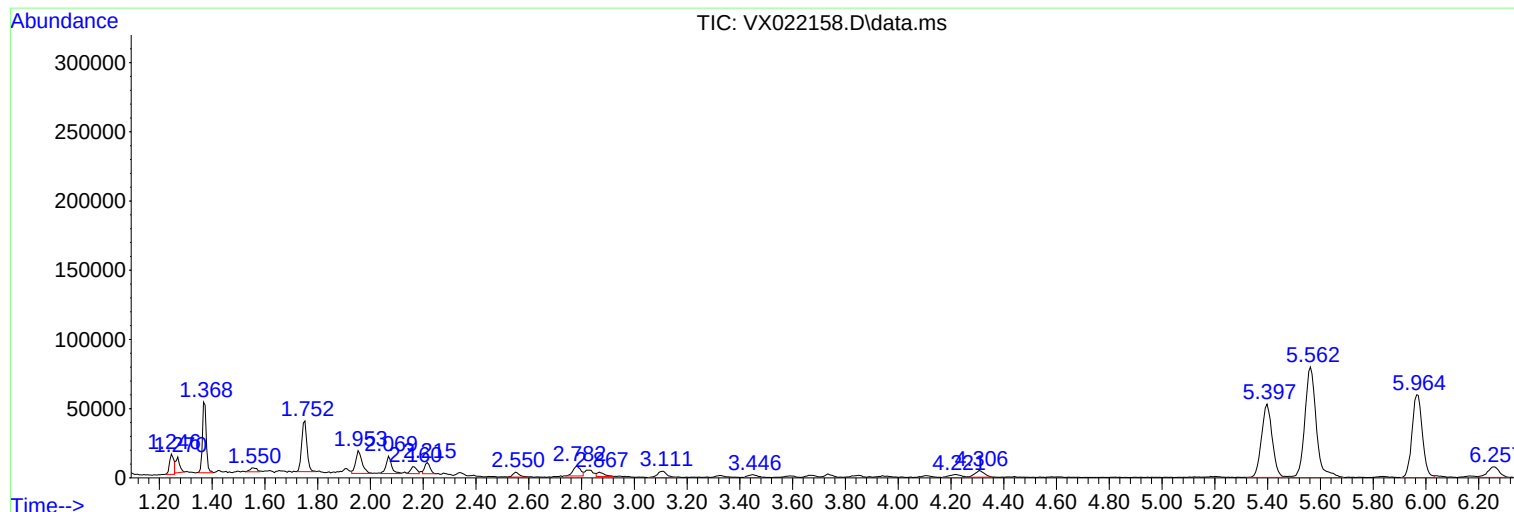
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Instrument :
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ClientSampleId :
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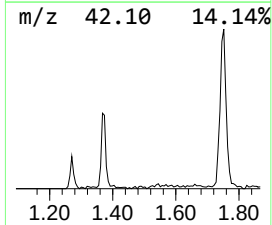
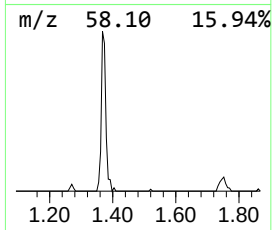
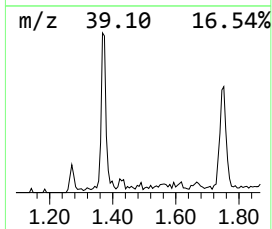
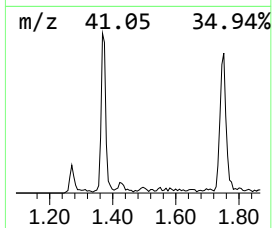
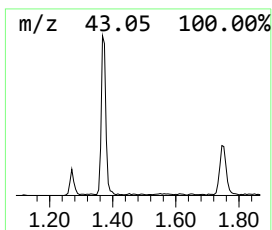
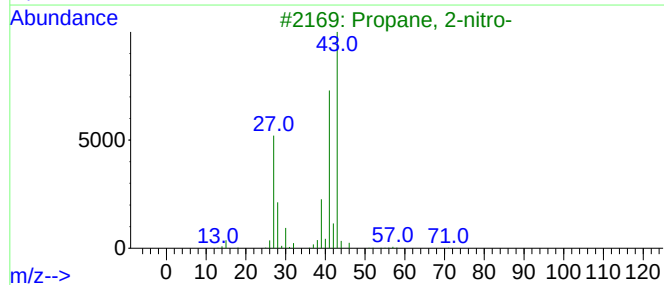
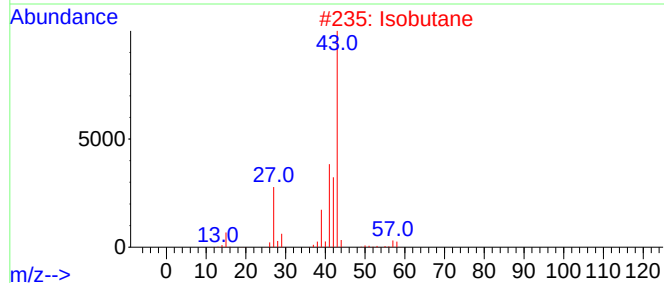
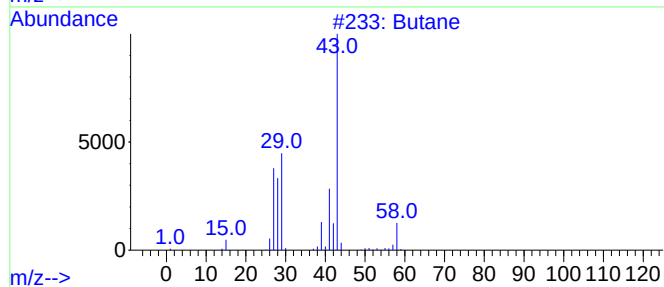
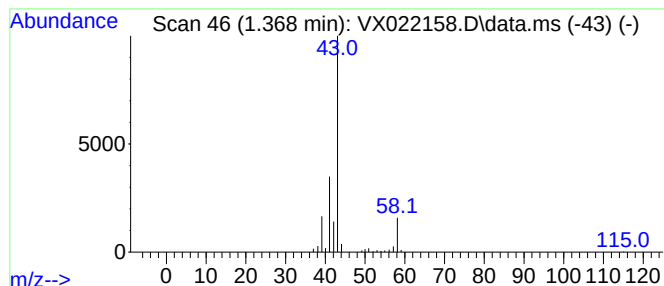
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.368	10.83 ug/l	51809	Pentafluorobenzene	5.562

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	Propane, 2-nitro-			89	C3H7NO2	000079-46-9	9
4	Propane, 1-nitro-			89	C3H7NO2	000108-03-2	9
5	Acetone			58	C3H6O	000067-64-1	4



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Instrument :
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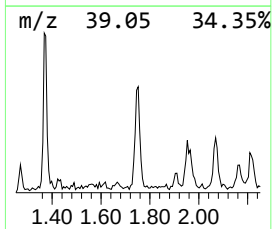
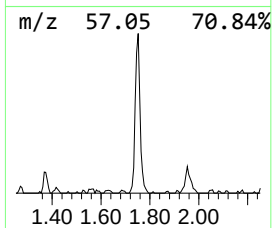
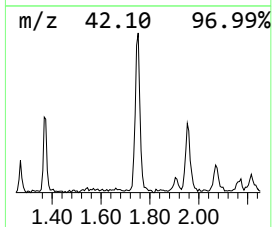
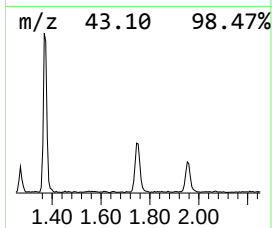
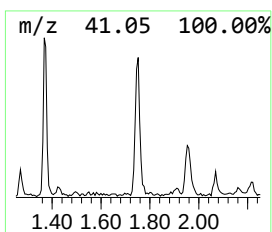
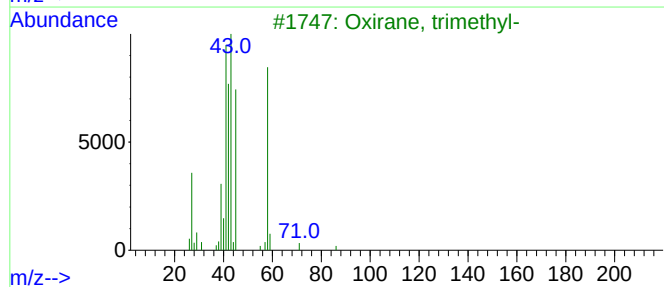
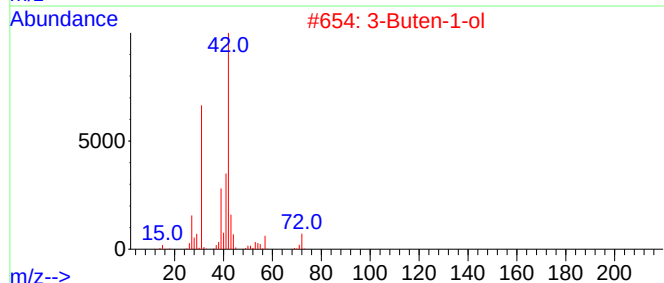
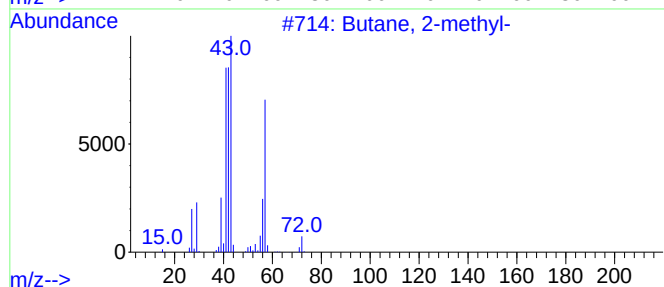
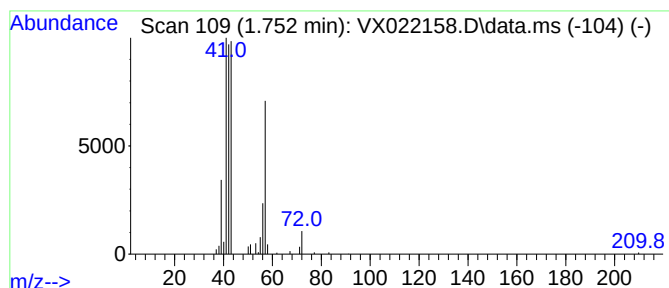
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Butane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	10.59 ug/l	50656	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	91
2			3-Buten-1-ol	72	C4H8O	000627-27-0	47
3			Oxirane, trimethyl-	86	C5H10O	005076-19-7	36
4			Pentane	72	C5H12	000109-66-0	33
5			2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	28



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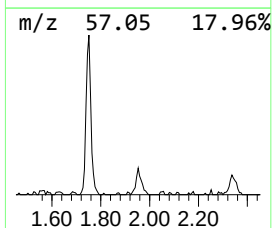
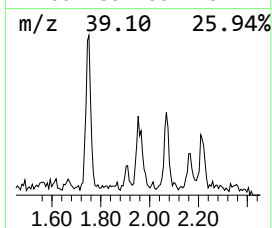
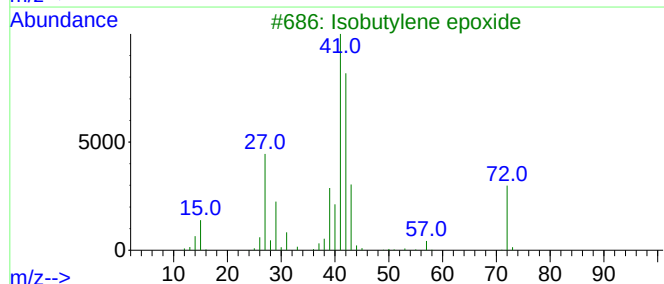
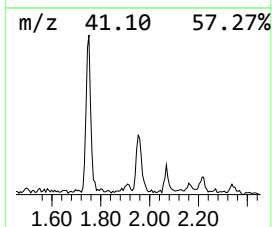
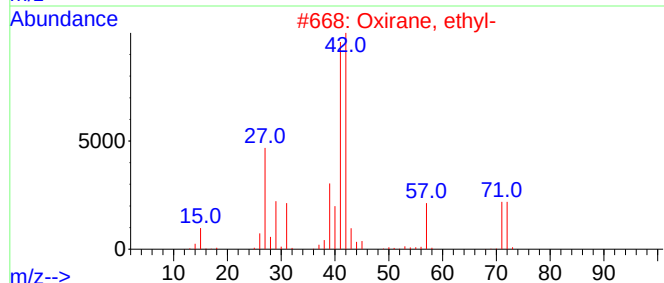
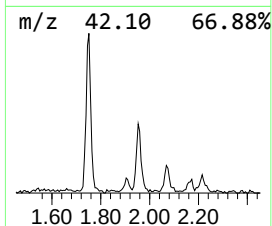
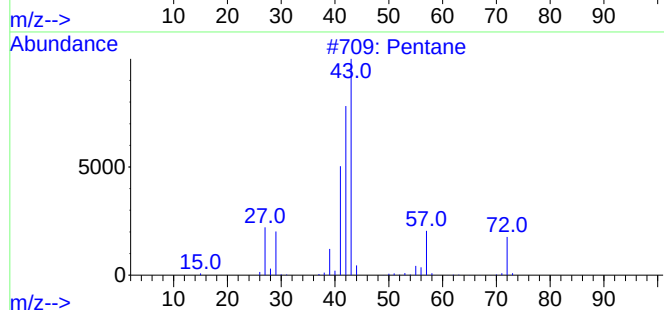
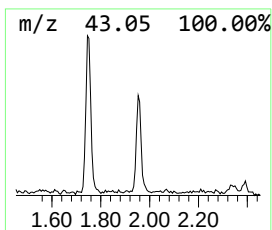
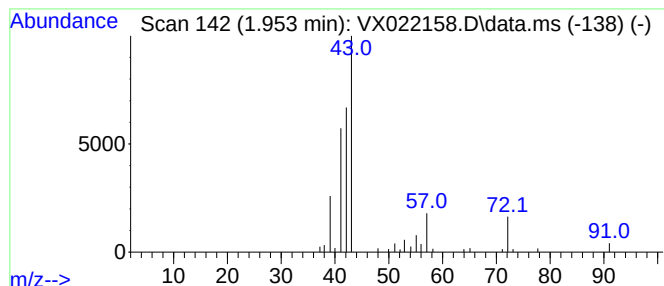
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.953	5.63 ug/l	26950	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	86
2			Oxirane, ethyl-	72	C4H8O	000106-88-7	43
3			Isobutylene epoxide	72	C4H8O	000558-30-5	38
4			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	36
5			Butane, 2-methyl-	72	C5H12	000078-78-4	33



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane	1.368	10.8	ug/l	51809	1	5.562	239278	50.0
Butane, 2-methyl-	1.752	10.6	ug/l	50656	1	5.562	239278	50.0
Pentane	1.953	5.6	ug/l	26950	1	5.562	239278	50.0