

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070325\
 Data File : VX046888.D
 Acq On : 03 Jul 2025 15:19
 Operator : JC/MD
 Sample : Q2465-02 100X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 62025-B

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\82X070225W.M
 Title : SW846 8260

Signal : TIC: VX046888.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.465	58	62	85	rVB	1827301	2378019	100.00%	12.888%
2	2.057	152	159	184	rBV	1208501	2214771	93.14%	12.003%
3	2.386	207	213	230	rBV	56530	112254	4.72%	0.608%
4	4.727	588	597	619	rBV	114292	383381	16.12%	2.078%
5	5.397	696	707	724	rBV3	225428	728719	30.64%	3.949%
6	5.562	724	734	757	rVB	379758	1176679	49.48%	6.377%
7	5.836	769	779	791	rBV	70781	214201	9.01%	1.161%
8	5.964	791	800	820	rVB	255654	728245	30.62%	3.947%
9	6.769	921	932	954	rBV	619302	1605838	67.53%	8.703%
10	8.647	1234	1240	1249	rBV	1324382	2166270	91.10%	11.741%
11	10.055	1465	1471	1487	rBV	1360637	1942329	81.68%	10.527%
12	11.079	1633	1639	1652	rBV	1223964	1529157	64.30%	8.288%
13	11.476	1700	1704	1709	rVB3	17335	25710	1.08%	0.139%
14	11.750	1746	1749	1759	rVB	23979	39975	1.68%	0.217%
15	12.018	1788	1793	1800	rBV	1641793	1985842	83.51%	10.763%
16	12.085	1801	1804	1813	rVB2	13498	29850	1.26%	0.162%
17	12.317	1838	1842	1848	rVB5	16427	30905	1.30%	0.167%
18	12.421	1853	1859	1863	rBV	40983	47126	1.98%	0.255%
19	12.969	1946	1949	1954	rVB5	18254	30306	1.27%	0.164%
20	13.164	1974	1981	1985	rBV4	13136	24015	1.01%	0.130%
21	13.262	1992	1997	2000	rBV	67757	90586	3.81%	0.491%
22	13.292	2000	2002	2007	rVB3	33793	41896	1.76%	0.227%
23	13.384	2012	2017	2019	rBV2	18892	26000	1.09%	0.141%
24	13.420	2019	2023	2026	rBV2	18181	24329	1.02%	0.132%
25	13.731	2071	2074	2077	rVV4	24096	31578	1.33%	0.171%
26	13.768	2077	2080	2087	rVV4	15224	32686	1.37%	0.177%
27	13.841	2087	2092	2099	rVB6	33876	62411	2.62%	0.338%
28	13.920	2099	2105	2110	rBV9	16310	36125	1.52%	0.196%
29	14.036	2120	2124	2127	rBV	101450	103710	4.36%	0.562%
30	14.225	2150	2155	2160	rVB3	39179	68656	2.89%	0.372%
31	14.475	2192	2196	2198	rBV3	31015	45728	1.92%	0.248%
32	14.560	2206	2210	2215	rVB5	19378	27997	1.18%	0.152%
33	14.609	2215	2218	2221	rBV2	60664	80387	3.38%	0.436%
34	14.670	2226	2228	2233	rVB5	21246	24807	1.04%	0.134%
35	14.756	2233	2242	2245	rBV	111132	151335	6.36%	0.820%
36	15.182	2308	2312	2313	rBV2	27914	33474	1.41%	0.181%

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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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Title : SW846 8260

37	15.207	2313	2316	2319	rVB	35853	42638	1.79%	0.231%
38	15.487	2357	2362	2367	rBV2	63498	96656	4.06%	0.524%
39	15.560	2370	2374	2378	rVV3	22237	36525	1.54%	0.198%

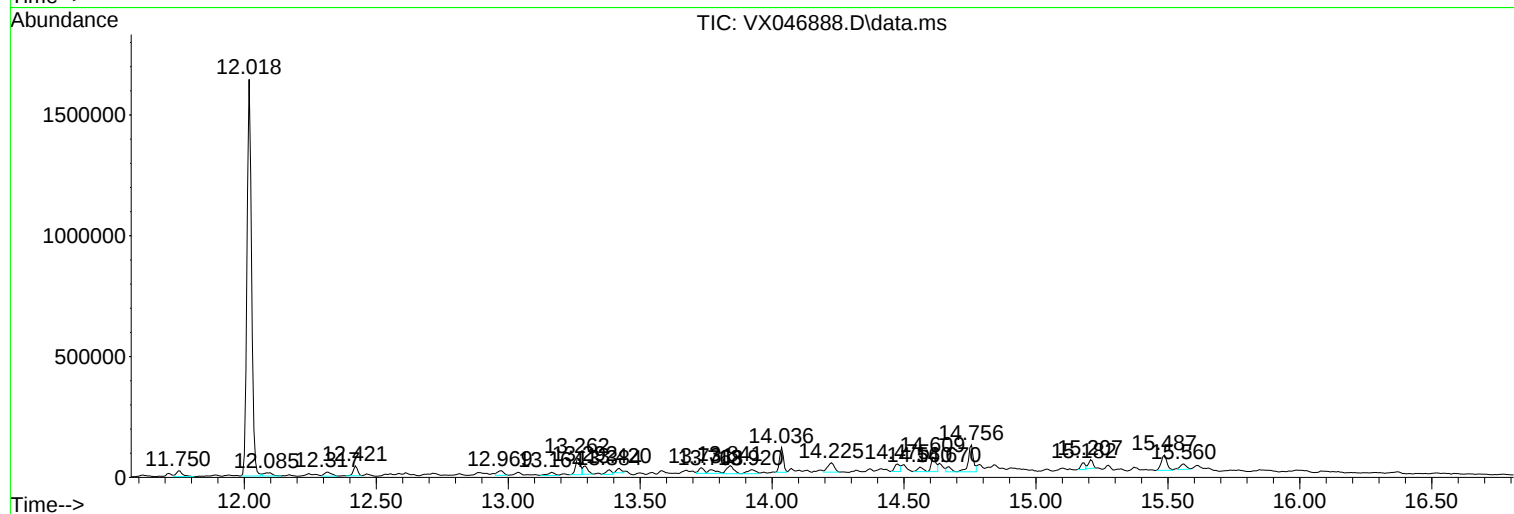
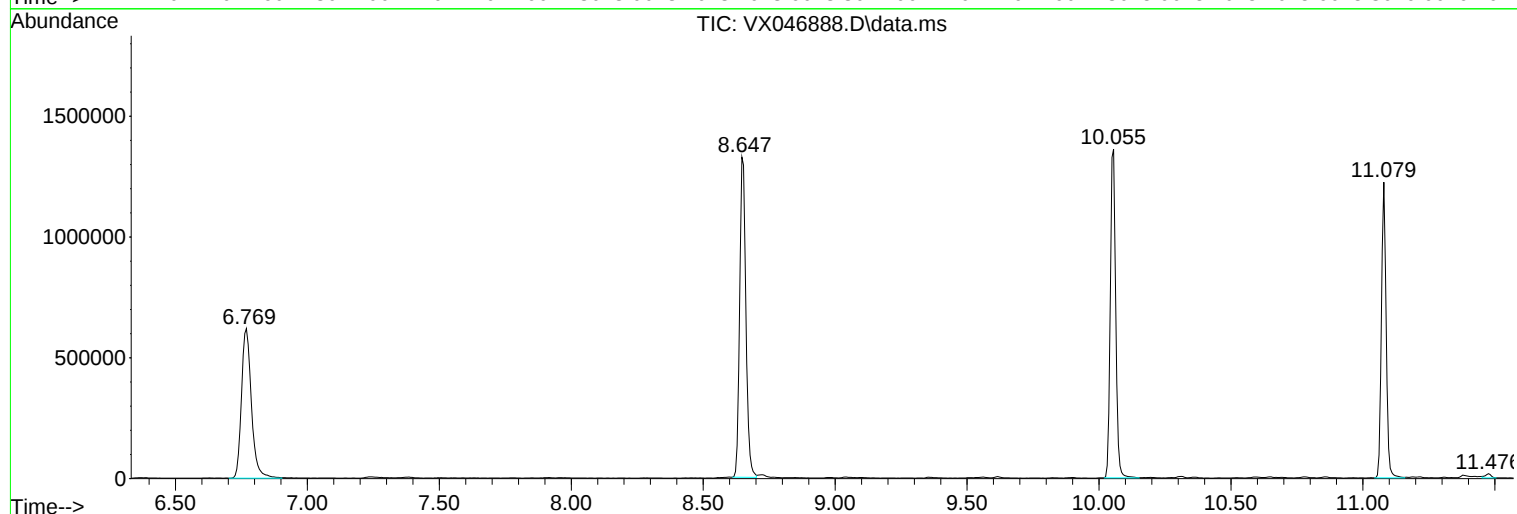
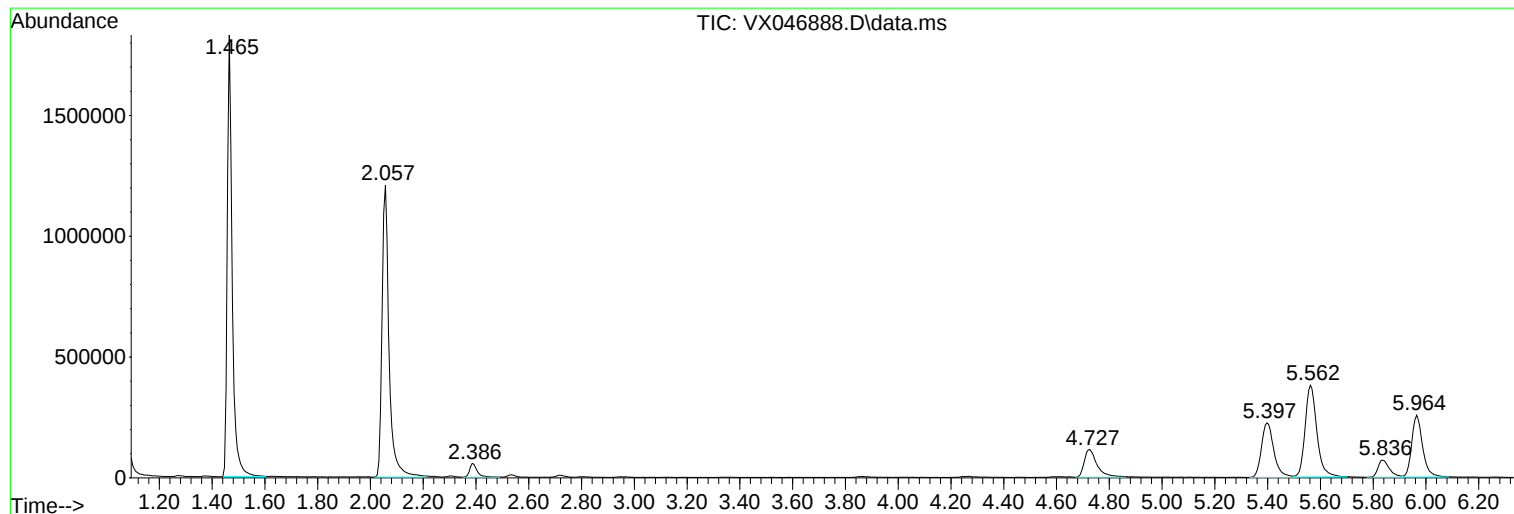
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070225W.M
Quant Title : SW846 8260

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



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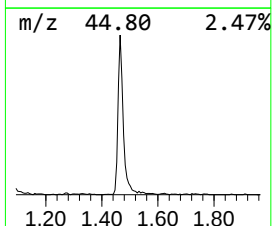
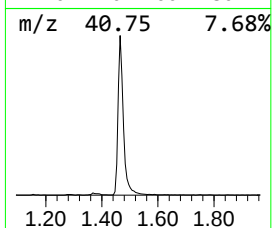
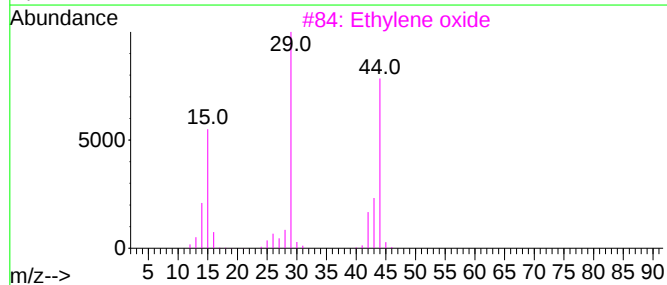
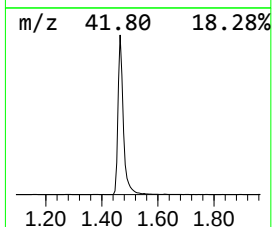
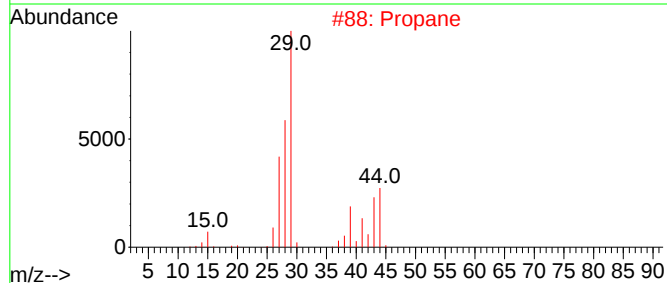
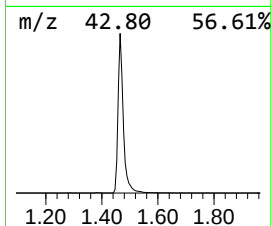
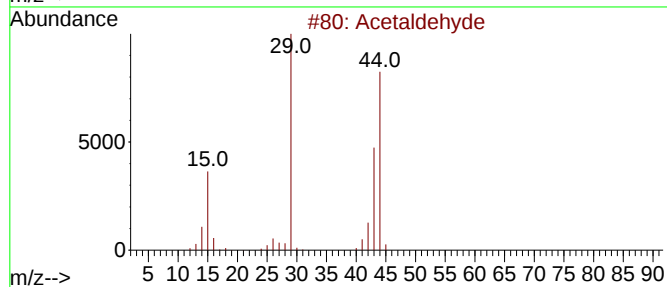
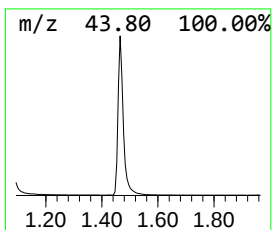
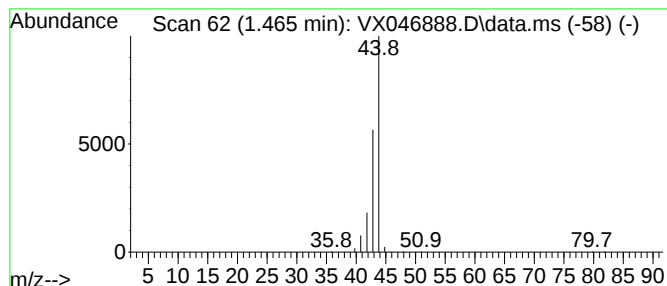
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070225W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown1.465 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.465	101.05 ug/l	2378020	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	9
2			Propane	44	C3H8	000074-98-6	5
3			Ethylene oxide	44	C2H4O	000075-21-8	5
4			Alanine	89	C3H7NO2	000056-41-7	4
5			Hydrogen isocyanate	43	CHNO	000075-13-8	3



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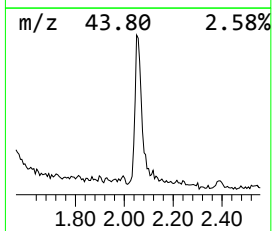
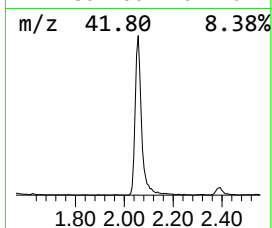
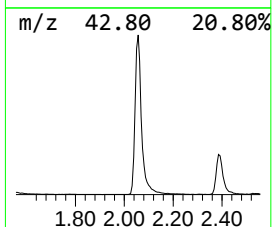
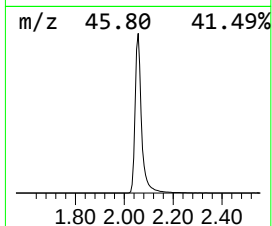
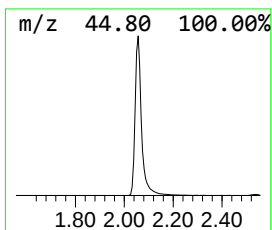
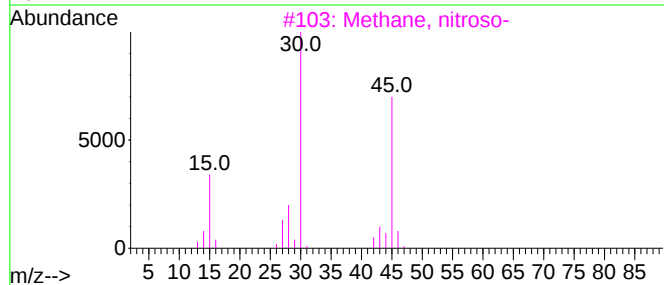
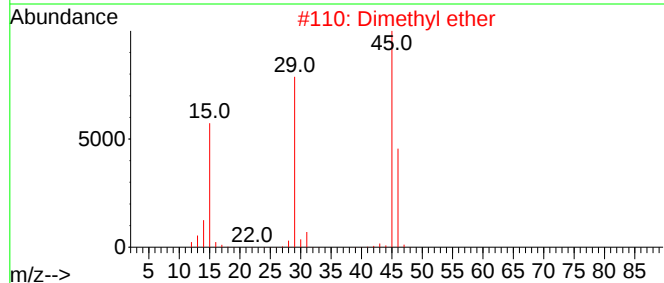
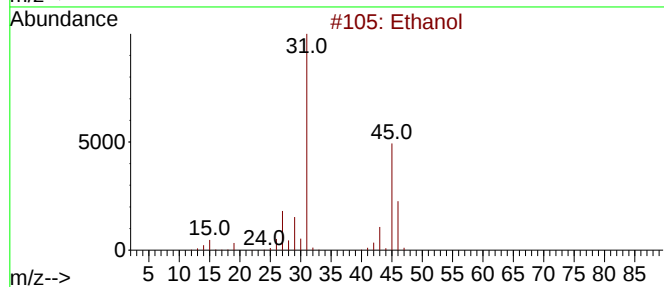
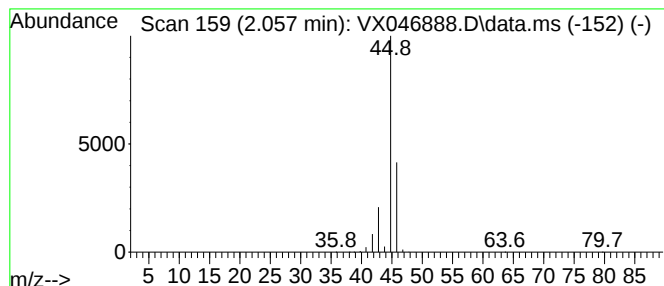
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Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.057	94.11 ug/l	2214770	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	83
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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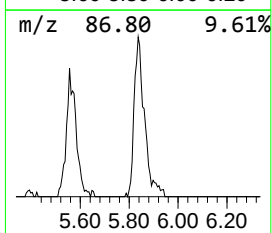
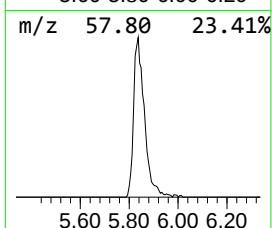
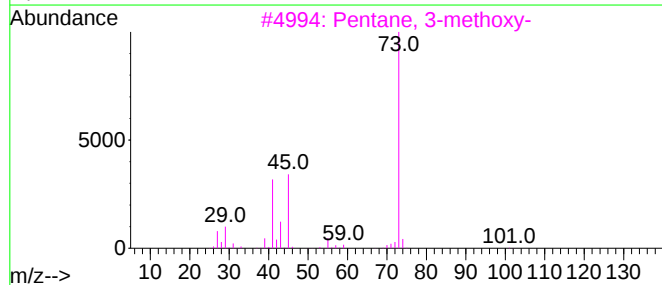
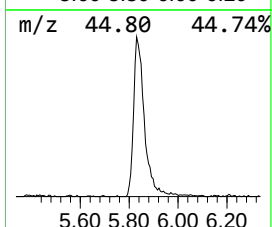
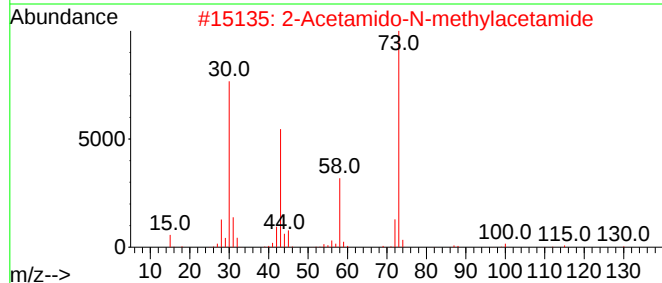
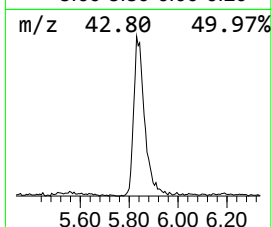
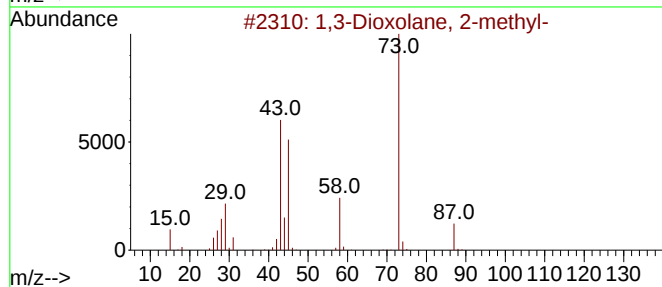
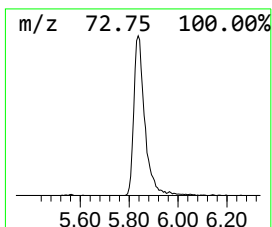
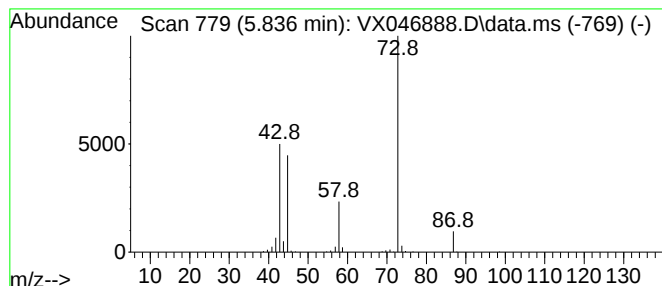
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070225W.M
Quant Title : SW846 8260

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

Peak Number 3 1,3-Dioxolane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.836	9.10 ug/l	214201	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	64
2			2-Acetamido-N-methylacetamide	130	C5H10N2O2	007606-79-3	37
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	28
4			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	17
5			N-Ethylformamide	73	C3H7NO	000627-45-2	12



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown1.465	1.465	101.1	ug/l	2378020	1	5.562	1176680	50.0
Ethanol	2.057	94.1	ug/l	2214770	1	5.562	1176680	50.0
1,3-Dioxolane, ...	5.836	9.1	ug/l	214201	1	5.562	1176680	50.0