

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
 Data File : VN070550.D
 Acq On : 10 Jan 2022 18:10
 Operator : JC/MD
 Sample : N1015-08
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 20987

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_N\methods\82N122721W.M
 Title : SW846 8260

Signal : TIC: VN070550.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.239	86	93	102	rBV3	37797	59093	1.17%	0.190%
2	4.143	779	803	837	rBV2	523360	1516088	30.09%	4.887%
3	4.291	841	858	886	rVB	91852	269760	5.35%	0.870%
4	4.586	947	968	995	rVB2	28507	93725	1.86%	0.302%
5	6.291	1583	1604	1630	rBV4	22232	74233	1.47%	0.239%
6	6.581	1687	1712	1751	rBV2	403502	1406160	27.91%	4.533%
7	7.067	1873	1893	1916	rBV4	72295	218322	4.33%	0.704%
8	7.340	1972	1995	2017	rBV	55103	156484	3.11%	0.504%
9	8.021	2225	2249	2260	rBV	663531	1607429	31.91%	5.181%
10	8.086	2260	2273	2301	rVB	1170245	2710445	53.80%	8.737%
11	8.437	2382	2404	2431	rBV	865118	2003384	39.77%	6.458%
12	8.837	2541	2553	2573	rVB	41353	96198	1.91%	0.310%
13	8.965	2582	2601	2628	rBV	1865572	3840960	76.24%	12.381%
14	9.164	2659	2675	2698	rBV4	25579	77415	1.54%	0.250%
15	9.411	2752	2767	2781	rBV2	67688	139388	2.77%	0.449%
16	9.542	2804	2816	2838	rVB3	17414	51071	1.01%	0.165%
17	10.293	3059	3096	3132	rBV6	66595	416239	8.26%	1.342%
18	10.440	3133	3151	3181	rBV	2648464	5037941	100.00%	16.239%
19	10.604	3200	3212	3232	rVB5	56204	120387	2.39%	0.388%
20	11.087	3376	3392	3401	rBV3	44481	86116	1.71%	0.278%
21	11.653	3592	3603	3613	rBV2	36026	62671	1.24%	0.202%
22	11.741	3613	3636	3663	rVV	2473825	4969490	98.64%	16.019%
23	12.731	3989	4005	4034	rBV	1763264	3140005	62.33%	10.122%
24	13.050	4114	4124	4138	rVB7	39332	72604	1.44%	0.234%
25	13.519	4288	4299	4318	rVB4	52376	95777	1.90%	0.309%
26	13.672	4340	4356	4379	rBV	1415769	2573428	51.08%	8.295%
27	13.769	4384	4392	4409	rVB2	74345	128062	2.54%	0.413%

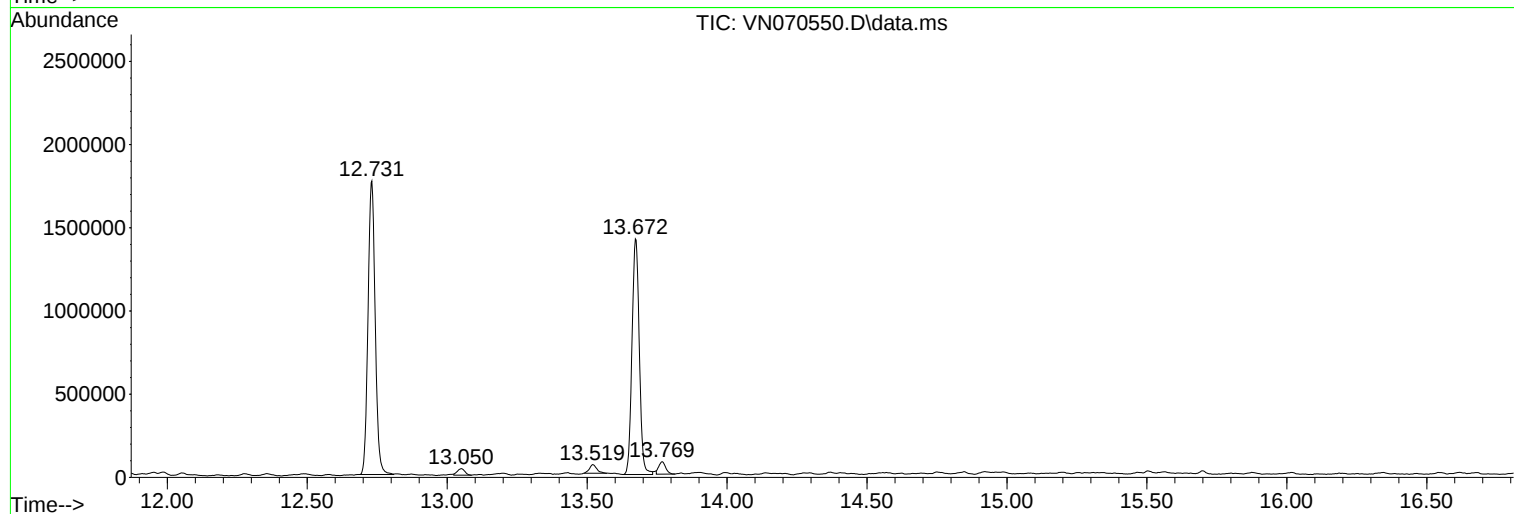
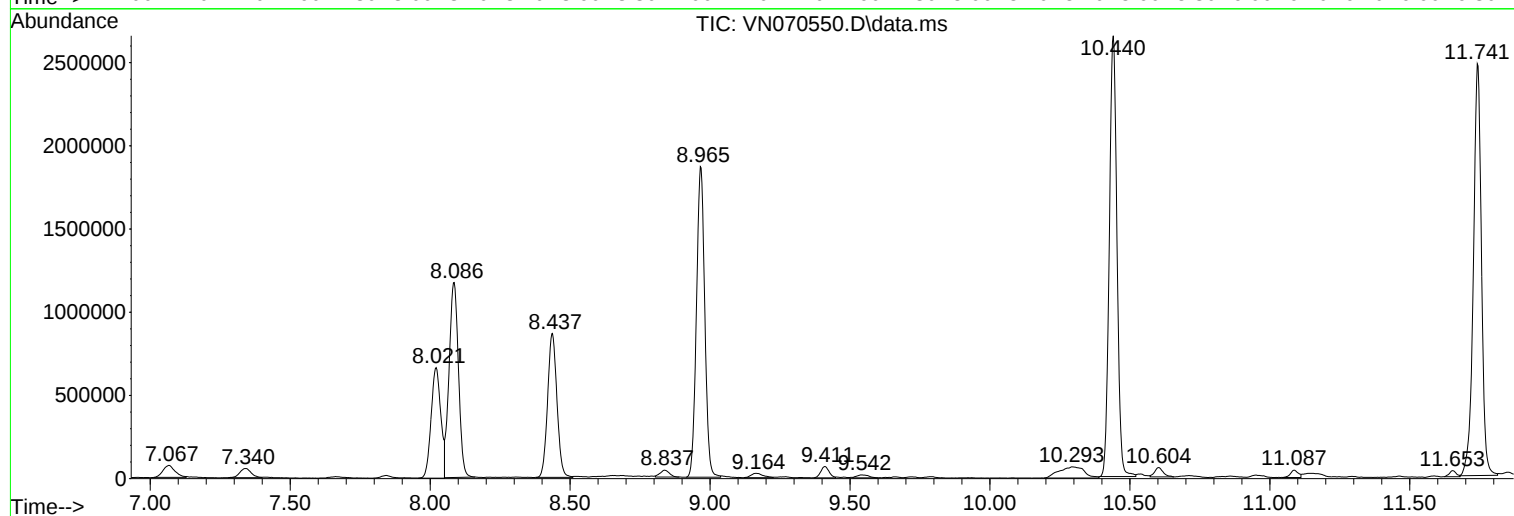
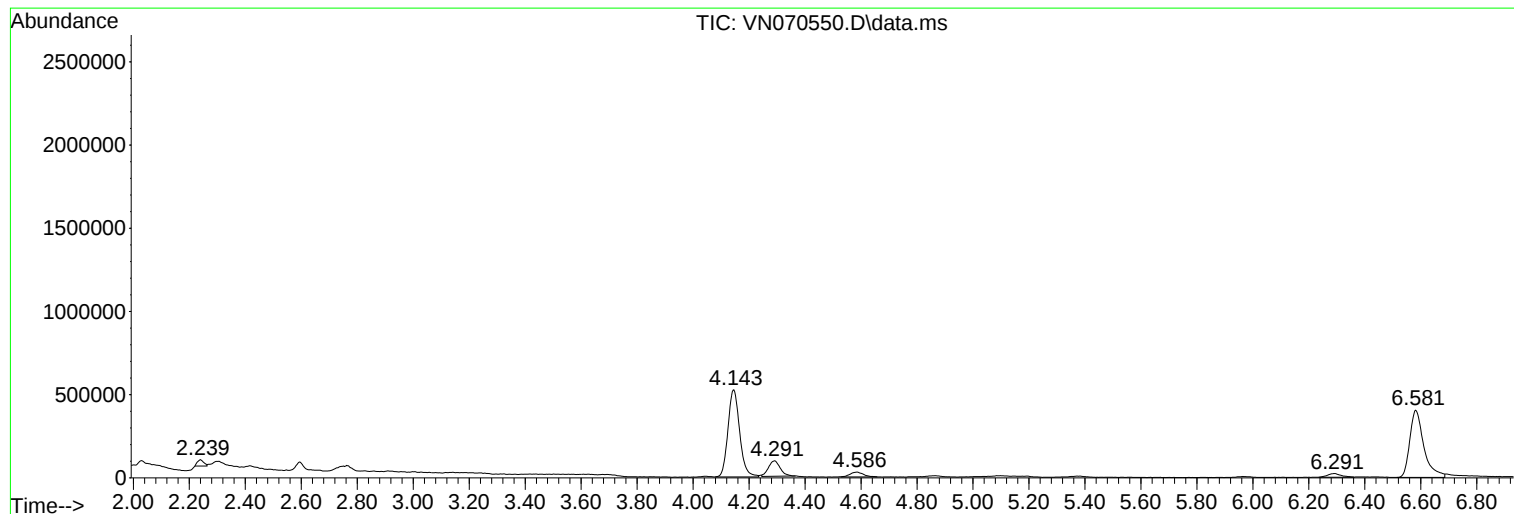
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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



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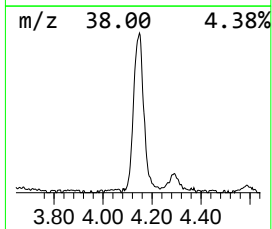
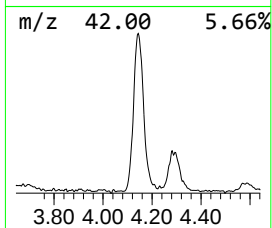
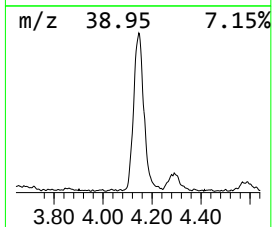
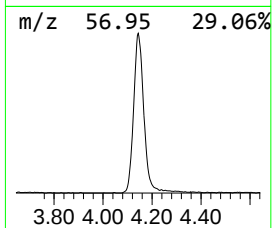
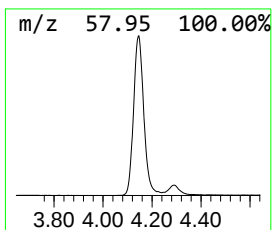
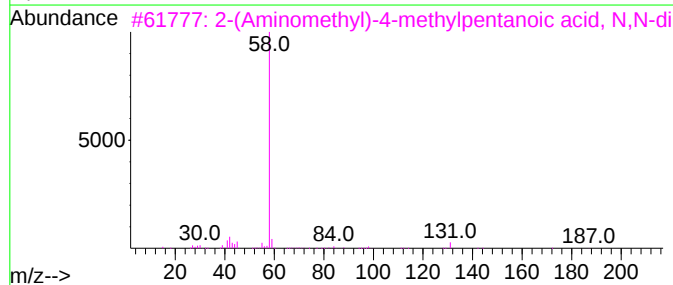
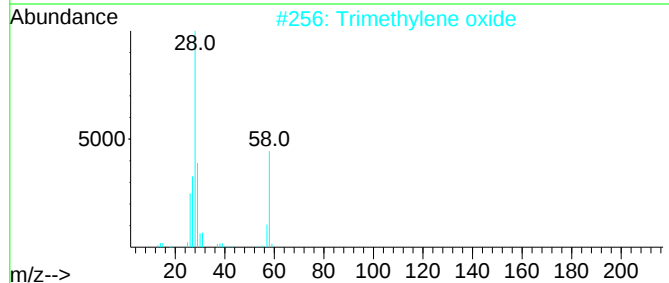
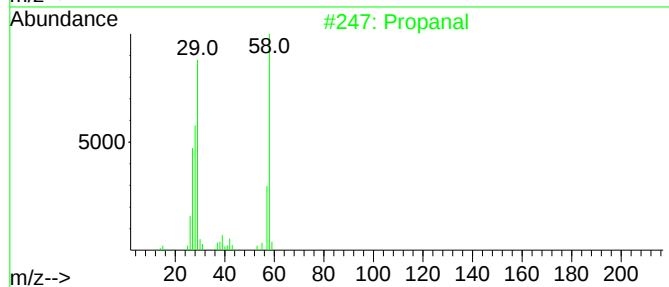
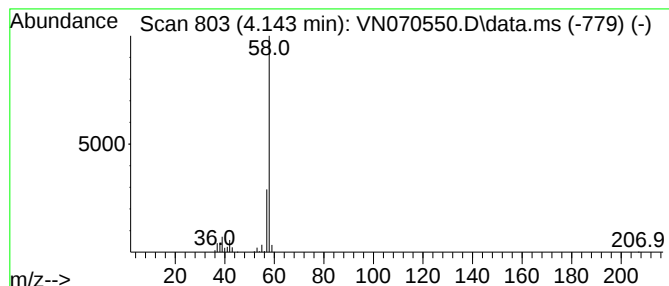
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 1 Propanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.143	27.97 ug/l	1516090	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal	58	C3H6O	000123-38-6	78
2			Trimethylene oxide	58	C3H6O	000503-30-0	9
3			2-(Aminomethyl)-4-methylpentanoic acid, N,N-di	187	C10H21NO2	1891211-54-3	9
4			Propylene oxide	58	C3H6O	000075-56-9	7
5			Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	5



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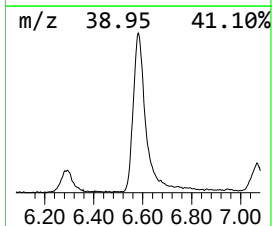
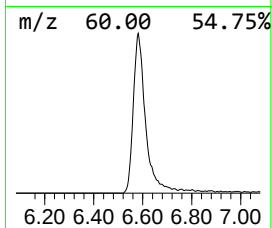
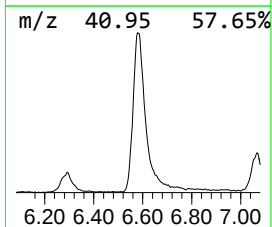
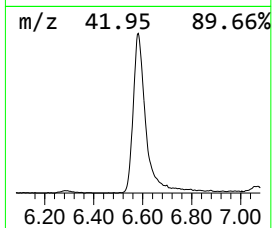
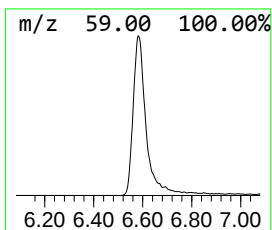
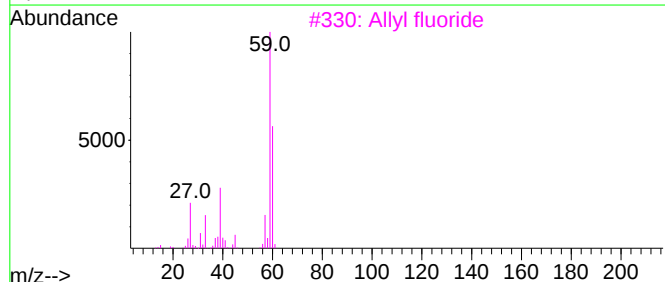
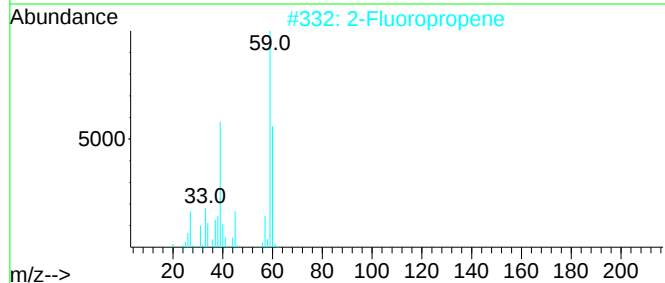
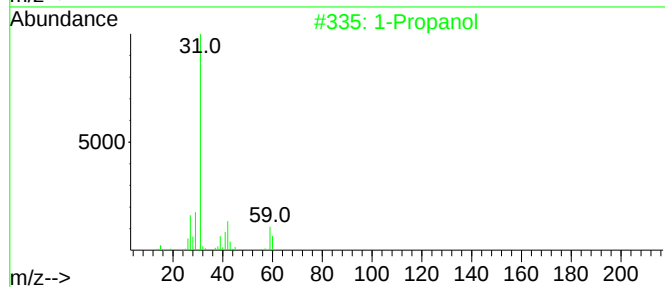
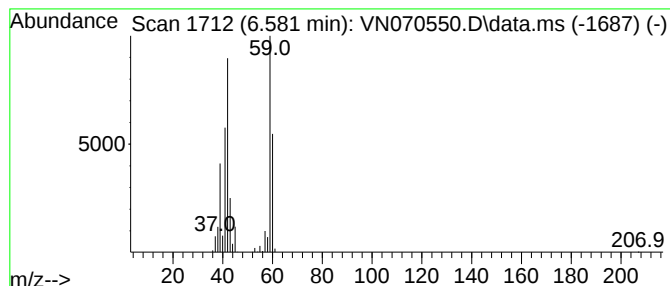
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Peak Number 2 1-Propanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.581	25.94 ug/l	1406160	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propanol	60	C3H8O	000071-23-8	59
2			2-Fluoropropene	60	C3H5F	001184-60-7	58
3			Allyl fluoride	60	C3H5F	000818-92-8	35
4			Cyclopropane	42	C3H6	000075-19-4	25
5			2-Butanol, 3-methoxy-	104	C5H12O2	053778-72-6	10



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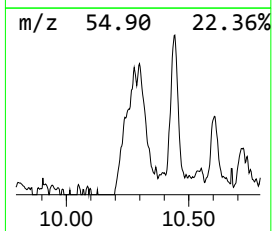
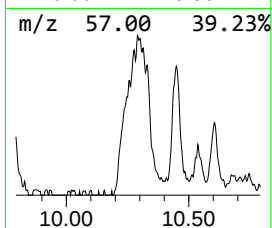
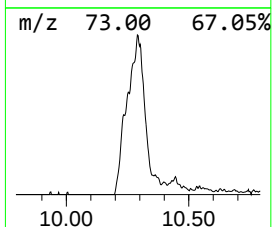
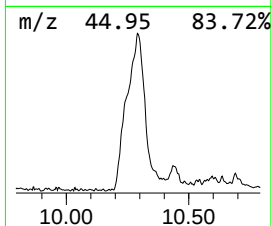
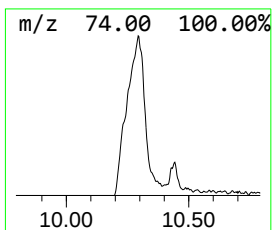
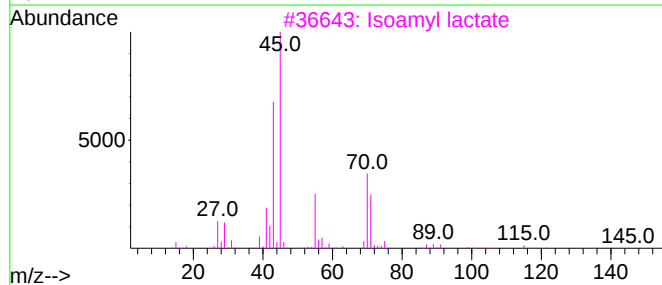
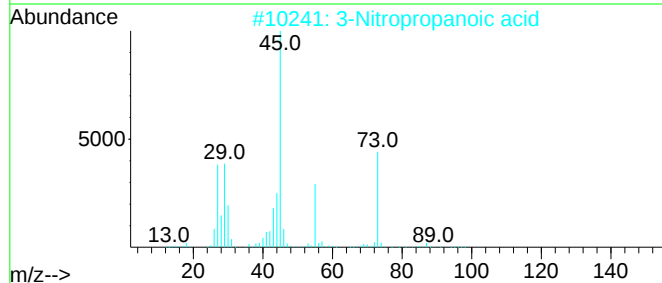
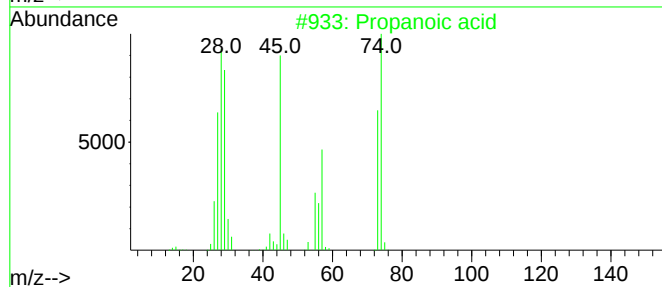
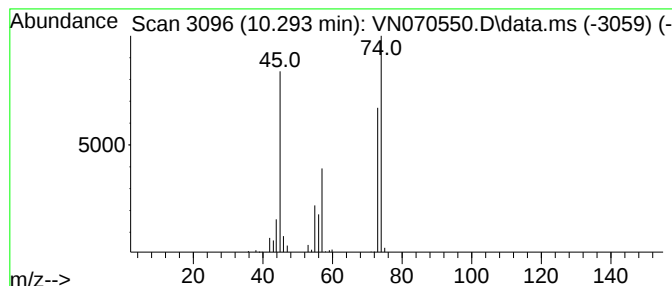
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Propanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.293	5.42 ug/l	416239	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid	74	C3H6O2	000079-09-4	90
2			3-Nitropropanoic acid	119	C3H5NO4	000504-88-1	25
3			Isoamyl lactate	160	C8H16O3	019329-89-6	9
4			1-Butaneboronic acid	102	C4H11BO2	004426-47-5	9
5			Ethanol, 2-nitro-	91	C2H5NO3	000625-48-9	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanal	4.143	28.0	ug/l	1516090	1	8.086	2710450	50.0
1-Propanol	6.581	25.9	ug/l	1406160	1	8.086	2710450	50.0
Propanoic acid	10.293	5.4	ug/l	416239	2	8.968	3840960	50.0