

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120222\
 Data File : VN075542.D
 Acq On : 02 Dec 2022 19:17
 Operator : JC\MD
 Sample : N5752-25
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TP-1

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\82N112122W.M

Title : SW846 8260

Signal : TIC: VN075542.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.295	35	41	54	rVB2	15980	48522	8.03%	1.171%
2	2.495	70	75	84	rBV5	13745	32820	5.43%	0.792%
3	2.824	124	131	137	rBV4	10377	31717	5.25%	0.765%
4	5.600	592	603	615	rVB4	24805	84266	13.95%	2.033%
5	6.689	775	788	802	rBV2	107921	363933	60.24%	8.781%
6	7.230	872	880	890	rVB4	6556	18428	3.05%	0.445%
7	7.447	908	917	919	rBV2	3482	7747	1.28%	0.187%
8	7.494	919	925	932	rVB3	7004	17928	2.97%	0.433%
9	8.171	1030	1040	1044	rBV	72795	167303	27.69%	4.037%
10	8.230	1044	1050	1061	rVB	195548	430976	71.34%	10.398%
11	8.606	1101	1114	1125	rBV4	95998	302996	50.16%	7.310%
12	9.106	1190	1199	1208	rBV	262190	532362	88.12%	12.844%
13	9.353	1233	1241	1250	rBV	36483	73974	12.24%	1.785%
14	10.571	1438	1448	1453	rBV	144745	263968	43.69%	6.369%
15	10.635	1453	1459	1466	rVB	78255	144123	23.86%	3.477%
16	11.871	1661	1669	1680	rBV	337118	604117	100.00%	14.576%
17	11.965	1680	1685	1691	rVB	8348	12117	2.01%	0.292%
18	12.071	1697	1703	1709	rBV2	16280	30558	5.06%	0.737%
19	12.406	1754	1760	1765	rVB3	5463	9786	1.62%	0.236%
20	12.853	1828	1836	1844	rBV	217302	374385	61.97%	9.033%
21	13.794	1988	1996	2005	rBV	326709	553100	91.56%	13.345%
22	14.170	2055	2060	2066	rBV2	7065	12173	2.02%	0.294%
23	14.241	2066	2072	2076	rVB3	5595	9416	1.56%	0.227%
24	14.612	2130	2135	2142	rBV3	6093	11852	1.96%	0.286%
25	14.764	2156	2161	2167	rBV3	3648	6133	1.02%	0.148%

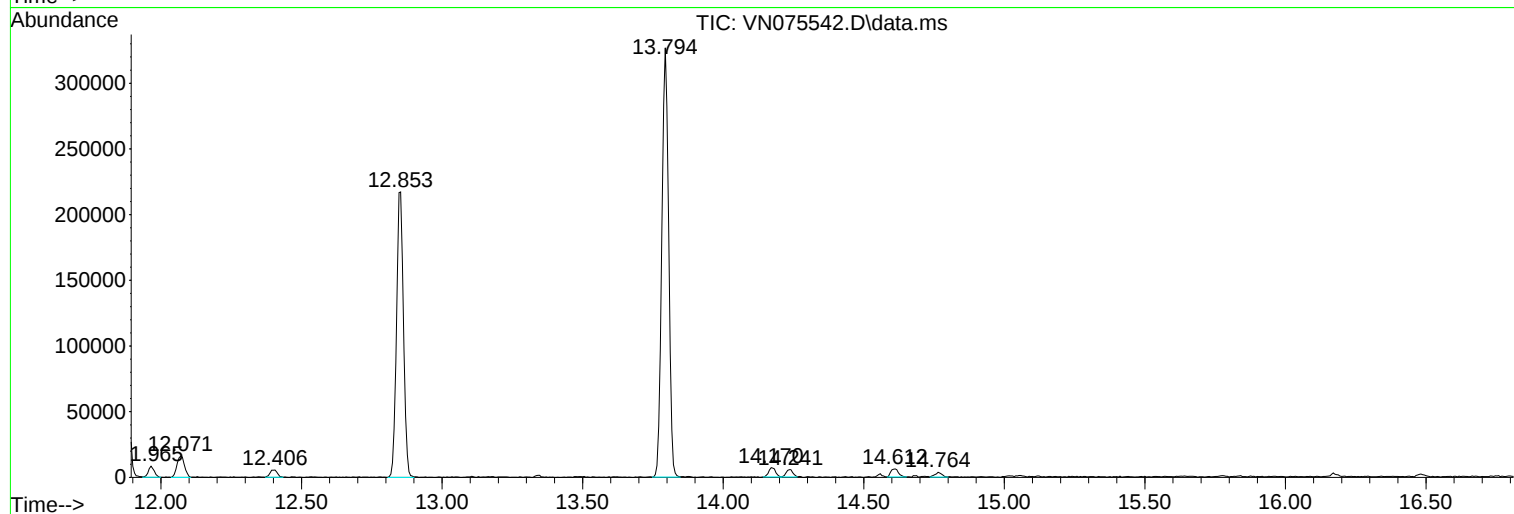
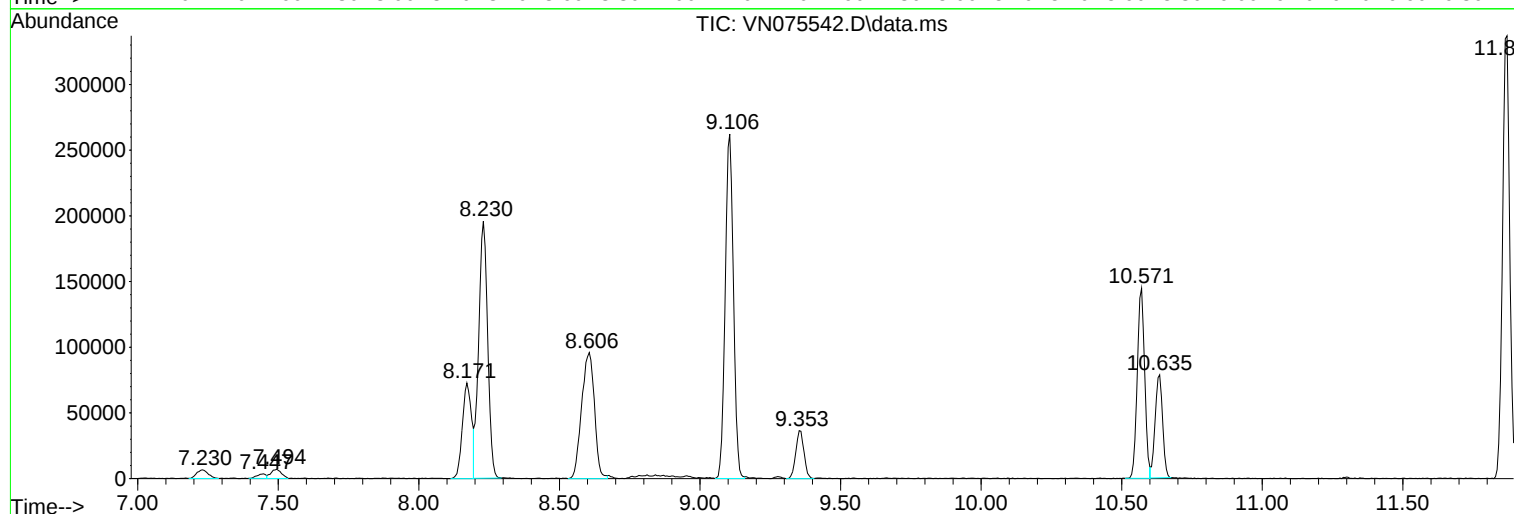
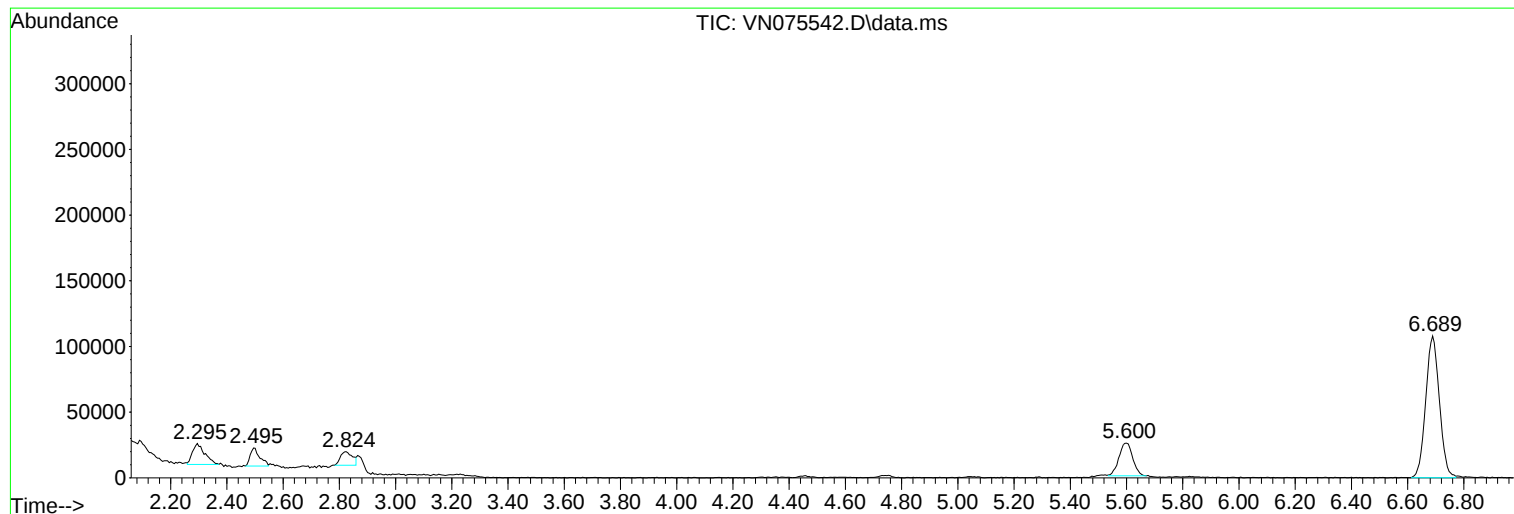
Sum of corrected areas: 4144700

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

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



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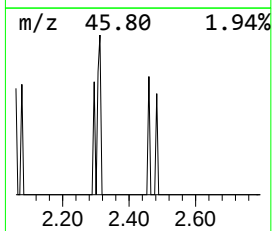
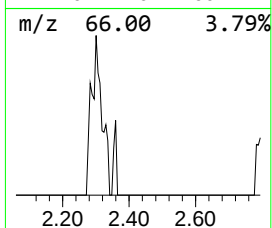
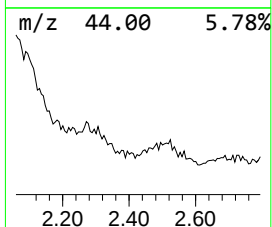
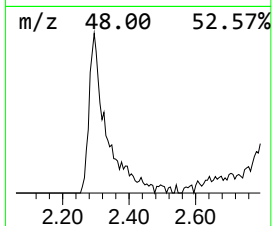
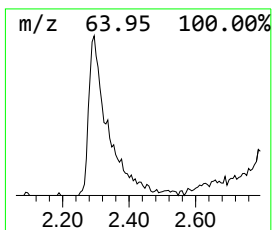
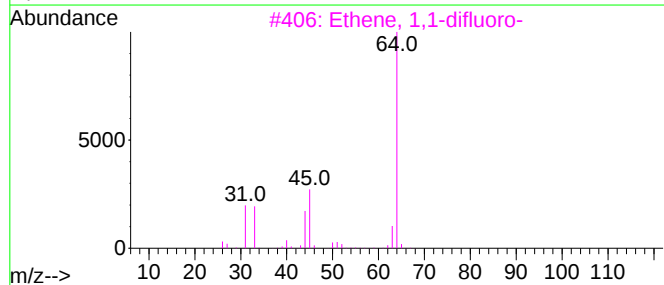
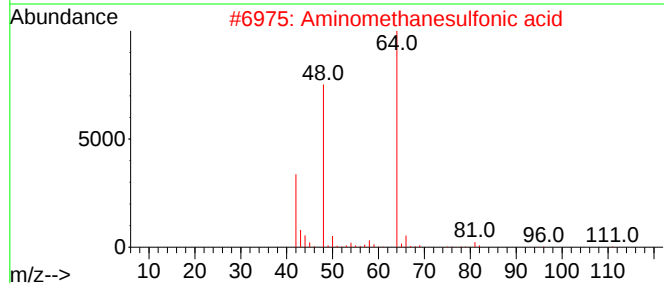
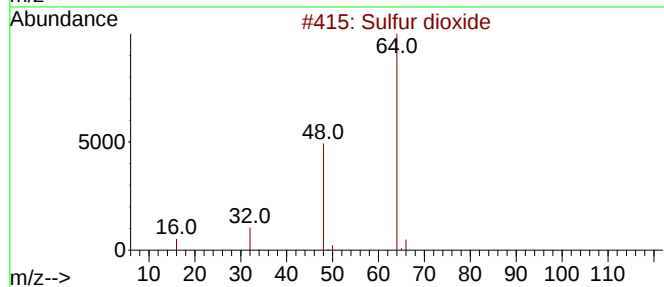
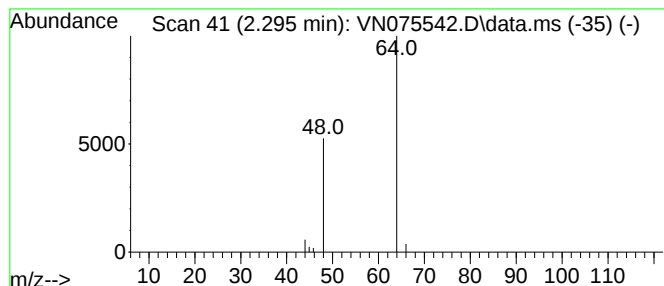
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.295	5.63 ug/l	48522	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
4			Ethyl Chloride	64	C2H5Cl	000075-00-3	3
5			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	3



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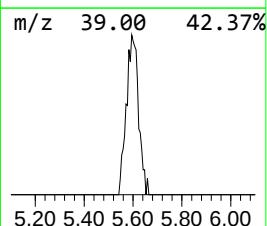
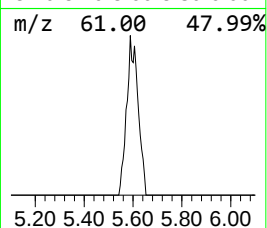
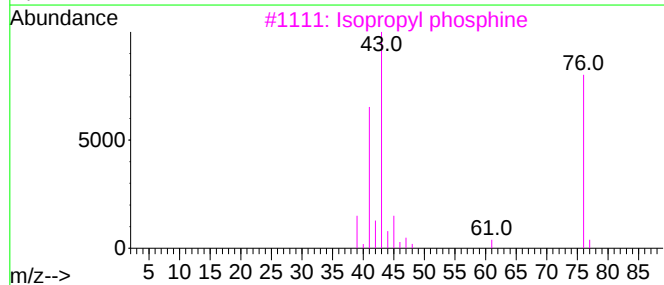
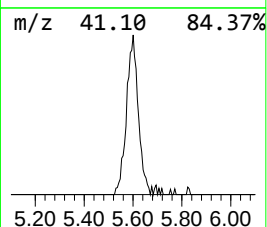
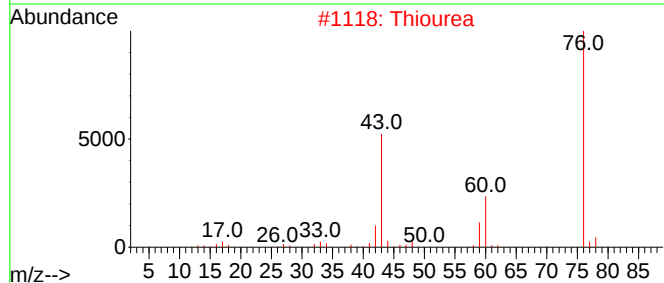
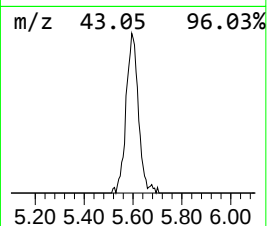
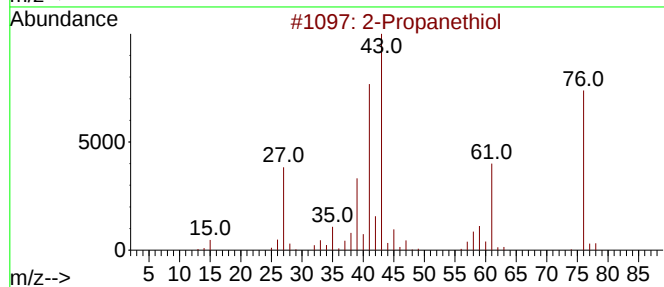
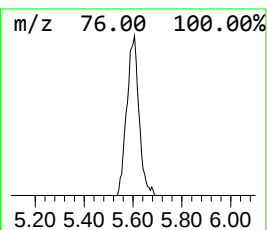
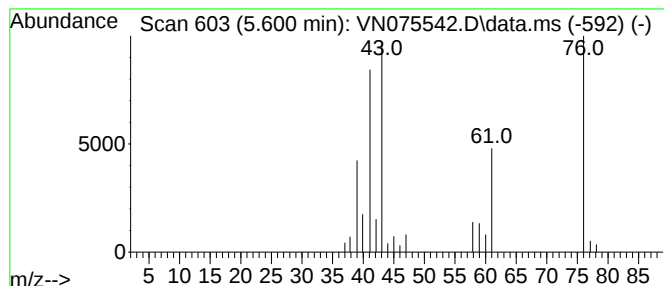
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Quant Title : SW846 8260

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

Peak Number 2 2-Propanethiol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.600	9.78 ug/l	84266	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanethiol	76	C3H8S	000075-33-2	90
2			Thiourea	76	CH4N2S	000062-56-6	59
3			Isopropyl phosphine	76	C3H9P	004538-29-8	45
4			Propyl mercaptan	76	C3H8S	000107-03-9	9
5			Propane, 1,3-dichloro-	112	C3H6Cl2	000142-28-9	9



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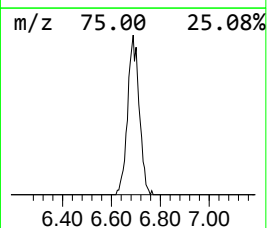
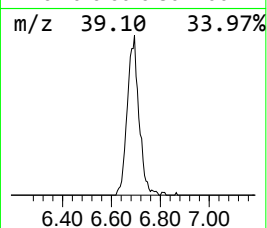
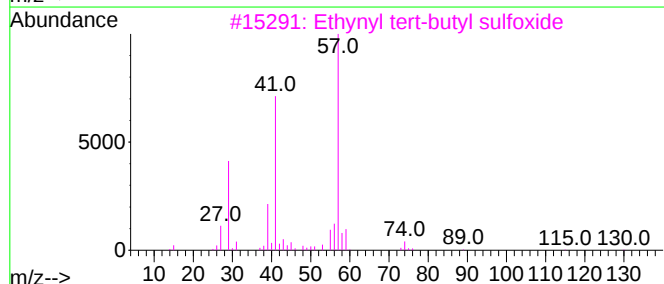
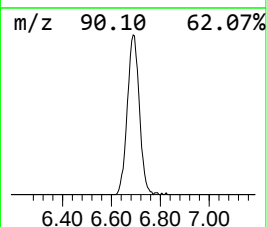
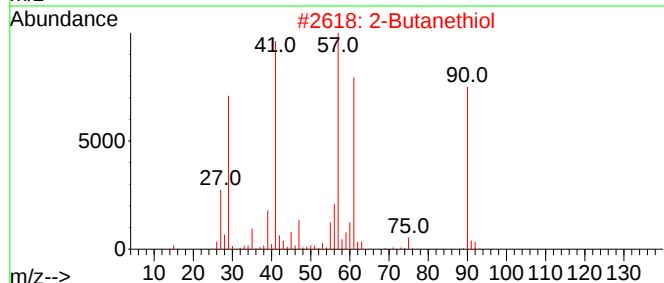
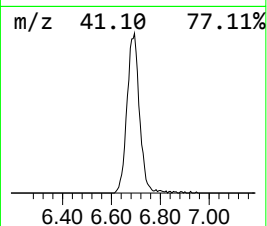
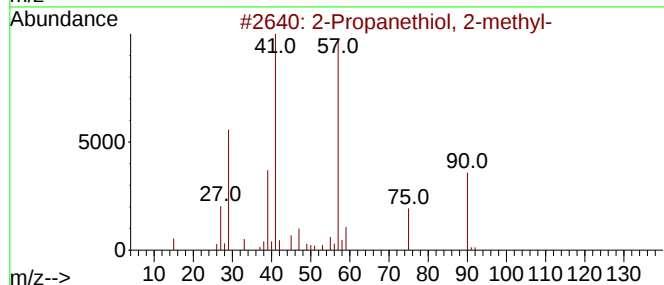
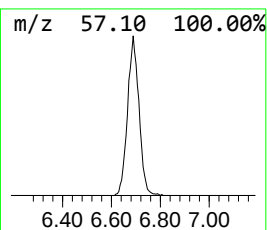
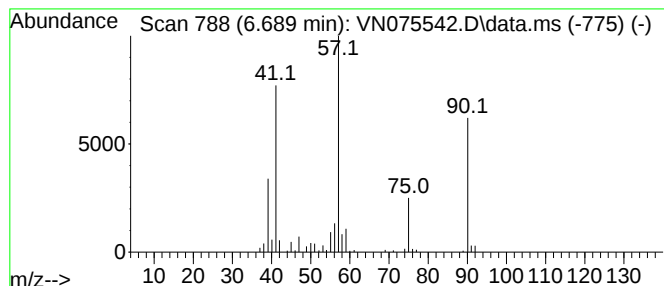
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.689	42.22 ug/l	363933	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	90
2			2-Butanethiol	90	C4H10S	000513-53-1	33
3			Ethynyl tert-butyl sulfoxide	130	C6H10OS	041463-34-7	25
4			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	14
5			Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	12



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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
Sulfur dioxide	2.295	5.6	ug/l	48522	1	8.230	430976	50.0
2-Propanethiol	5.600	9.8	ug/l	84266	1	8.230	430976	50.0
2-Propanethiol,...	6.689	42.2	ug/l	363933	1	8.230	430976	50.0