

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122820\
 Data File : VN065283.D
 Acq On : 28 Dec 2020 14:02
 Operator : JC/MD
 Sample : L5218-01
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-1R

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\82N122220W.M
 Title : Sw846 8260

Signal : TIC: VN065283.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.148	117	127	139	rBV3	13478	22472	1.80%	0.292%
2	2.965	370	381	396	rVB	18055	36419	2.92%	0.473%
3	4.785	924	947	974	rBV4	33590	114560	9.20%	1.489%
4	5.004	998	1015	1037	rVB4	12121	45609	3.66%	0.593%
5	5.904	1268	1295	1324	rBV2	199092	710563	57.06%	9.236%
6	7.553	1788	1808	1819	rBV2	157632	395714	31.78%	5.143%
7	7.627	1819	1831	1854	rVB	264579	630951	50.67%	8.201%
8	7.991	1927	1944	1960	rBV2	156022	363675	29.20%	4.727%
9	8.074	1962	1970	1983	rVB4	10769	23803	1.91%	0.309%
10	8.550	2103	2118	2143	rBV	413332	868097	69.71%	11.283%
11	10.058	2572	2587	2613	rBV	675155	1245257	100.00%	16.186%
12	11.380	2984	2998	3031	rBV	667496	1190180	95.58%	15.470%
13	12.376	3295	3308	3330	rBV	531425	936707	75.22%	12.175%
14	13.318	3587	3601	3632	rBV	549331	987546	79.30%	12.836%
15	13.695	3707	3718	3729	rBV4	17802	29283	2.35%	0.381%
16	13.765	3729	3740	3754	rVB3	7664	13929	1.12%	0.181%
17	14.132	3842	3854	3870	rBV2	11394	22825	1.83%	0.297%
18	14.286	3894	3902	3912	rVB	16592	26541	2.13%	0.345%
19	15.530	4281	4289	4298	rVB3	10286	15183	1.22%	0.197%
20	15.752	4351	4358	4371	rVB2	9415	14274	1.15%	0.186%

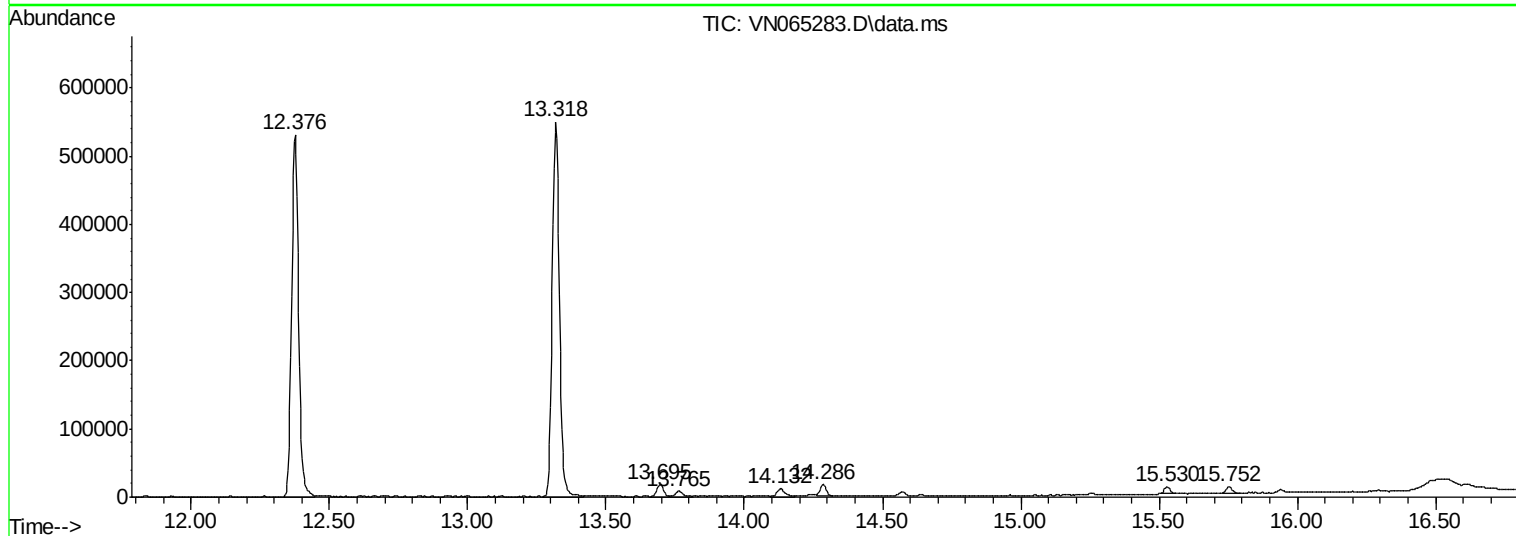
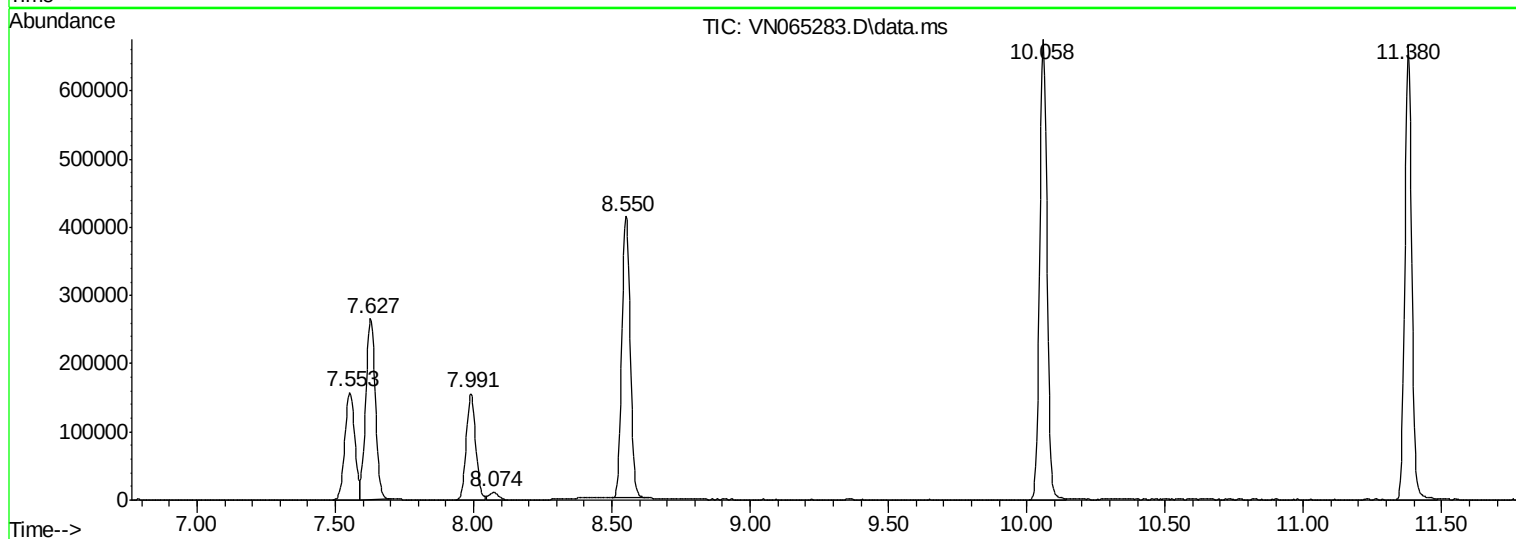
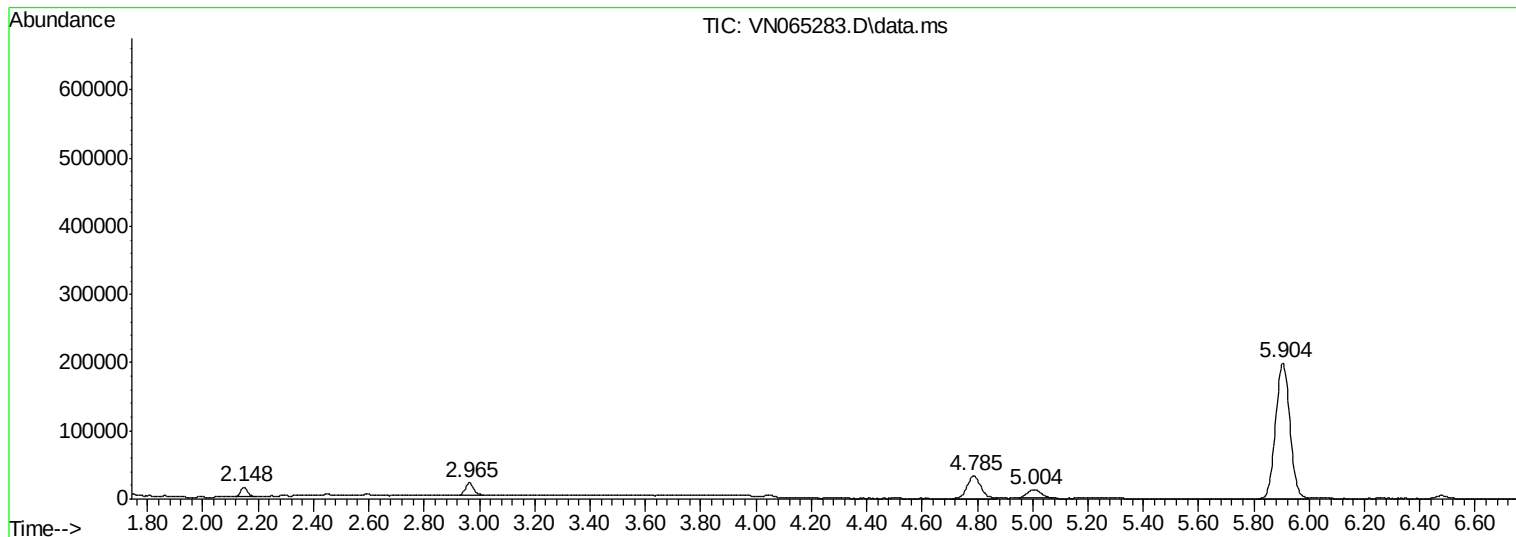
Sum of corrected areas: 7693588

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Quant Title : SW846 8260

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



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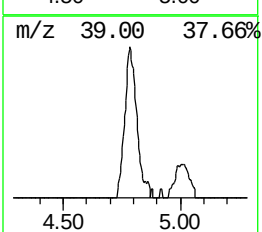
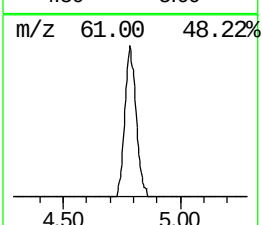
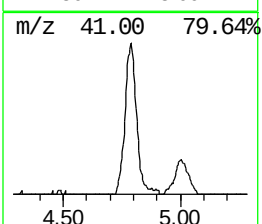
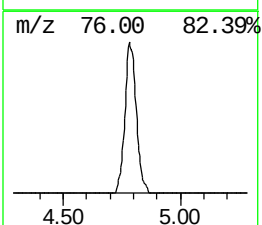
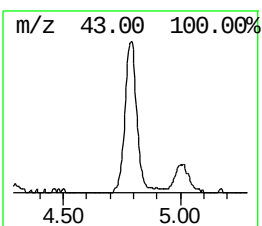
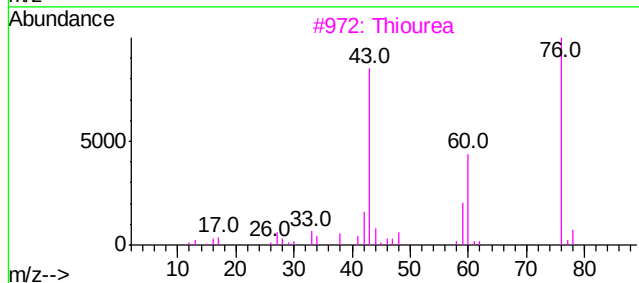
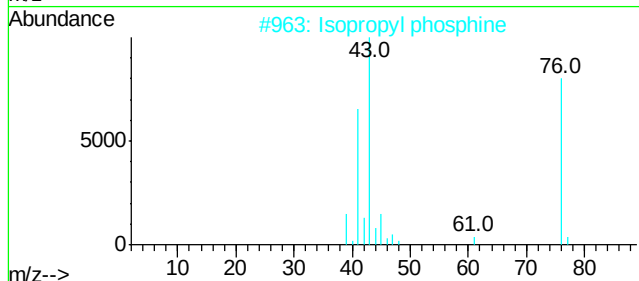
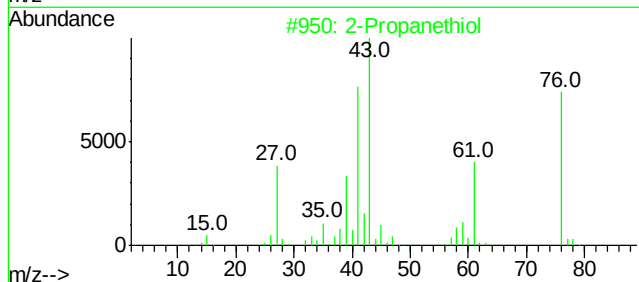
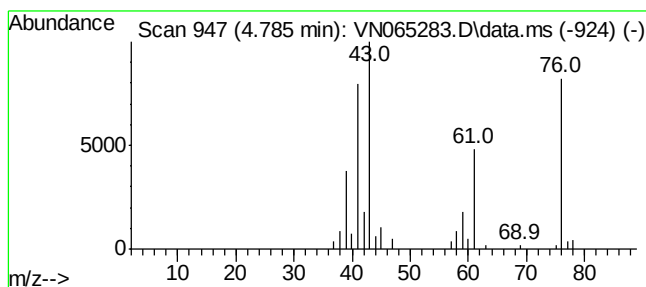
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220w.M
Quant Title : SW846 8260

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

Peak Number 1 2-Propanethiol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.785	9.08 ug/l	114560	Pentafluorobenzene	7.627

Hit# of 5	Tentative ID	Mw	MolForm	CAS#	Qual
1	2-Propanethiol	76	C3H8S	000075-33-2	91
2	Isopropyl phosphine	76	C3H9P	004538-29-8	72
3	Thiourea	76	CH4N2S	000062-56-6	39
4	Propyl mercaptan	76	C3H8S	000107-03-9	9
5	1-Propene, 2-chloro-	76	C3H5Cl	000557-98-2	4



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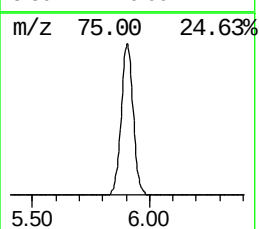
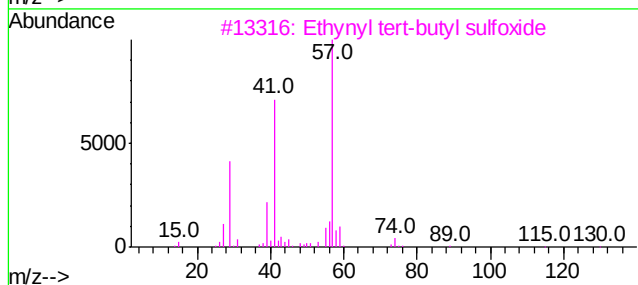
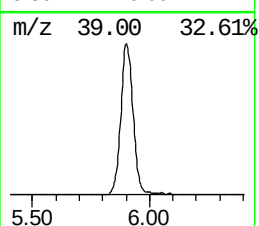
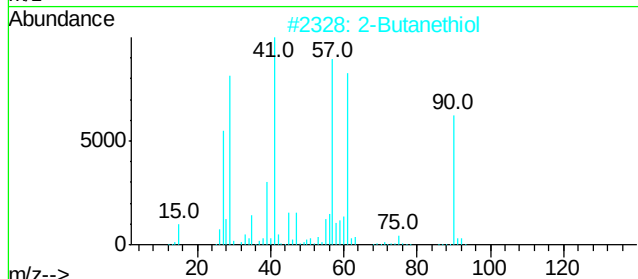
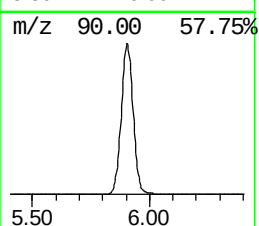
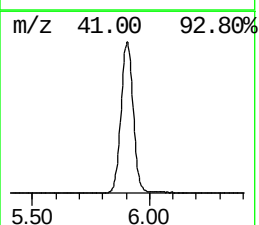
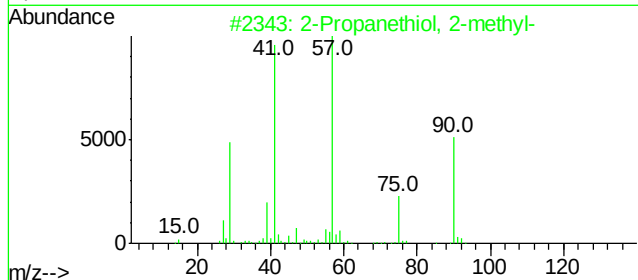
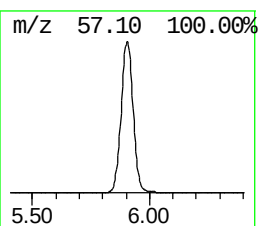
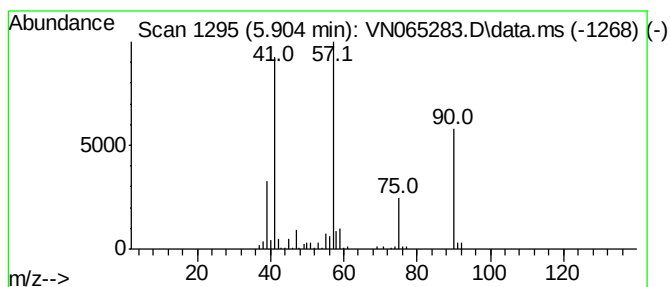
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.904	56.31 ug/l	710563	Pentafluorobenzene	7.627

Hit# of 5	Tentative ID	Mw	MolForm	CAS#	Qual
1	2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	91
2	2-Butanethiol	90	C4H10S	000513-53-1	42
3	Ethynyl tert-butyl sulfoxide	130	C6H10OS	041463-34-7	16
4	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	14
5	Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Propanethiol	4.785	9.1	ug/l	114560	1	7.627	630951	50.0
2-Propanethiol,...	5.904	56.3	ug/l	710563	1	7.627	630951	50.0