

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY081021\
 Data File : VY005588.D
 Acq On : 10 Aug 2021 12:20
 Operator : SY/MD
 Sample : M3328-03
 Misc : 7.34G/5ML/MSVOA_Y/SOIL
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 20210474-60

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_Y\methods\82Y080221S.M
 Title : SW846 8260

Signal : TIC: VY005588.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.863	4	7	17	rVB2	21022	38453	1.56%	0.400%
2	3.954	341	350	357	rBV	26335	72294	2.93%	0.753%
3	4.040	357	364	381	rVV3	22357	66116	2.68%	0.689%
4	4.204	381	391	405	rVB	12051	33767	1.37%	0.352%
5	4.729	464	477	496	rBV4	21966	86630	3.52%	0.902%
6	7.003	839	850	865	rBV	16428	57124	2.32%	0.595%
7	7.728	957	969	974	rBV	172213	417688	16.95%	4.350%
8	7.795	974	980	991	rVB	290548	647943	26.30%	6.748%
9	8.149	1028	1038	1052	rVB	191092	419468	17.03%	4.369%
10	8.697	1119	1128	1138	rVB	468962	914566	37.12%	9.525%
11	10.185	1363	1372	1380	rBV	784037	1326732	53.85%	13.818%
12	11.490	1579	1586	1596	rBV	752157	1220823	49.55%	12.715%
13	12.489	1739	1750	1758	rBV2	1402829	2463735	100.00%	25.660%
14	12.843	1797	1808	1813	rBV3	18298	51347	2.08%	0.535%
15	13.069	1841	1845	1851	rVB2	22296	36173	1.47%	0.377%
16	13.282	1871	1880	1886	rBV	50192	91842	3.73%	0.957%
17	13.343	1886	1890	1896	rVV6	12045	26515	1.08%	0.276%
18	13.428	1896	1904	1909	rVV	795311	1235507	50.15%	12.868%
19	13.477	1909	1912	1920	rVB	40043	81354	3.30%	0.847%
20	13.642	1931	1939	1944	rBV5	14025	30046	1.22%	0.313%
21	13.965	1986	1992	2002	rVB	151527	251573	10.21%	2.620%
22	14.391	2056	2062	2071	rBV5	10430	31631	1.28%	0.329%

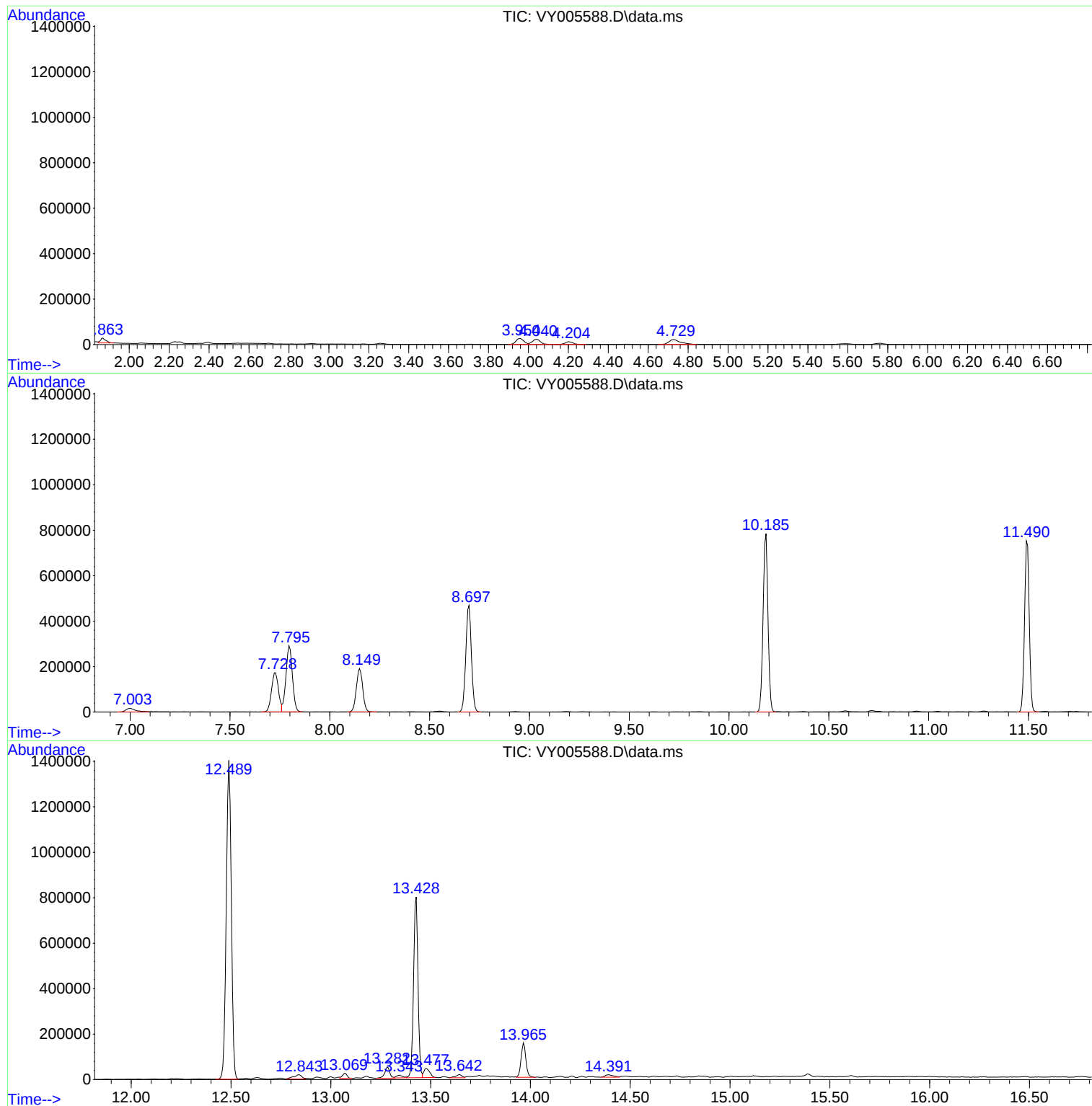
Sum of corrected areas: 9601327

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y080221S.M
Quant Title : SW846 8260

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



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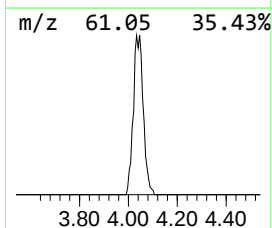
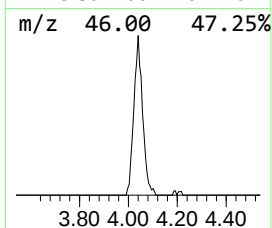
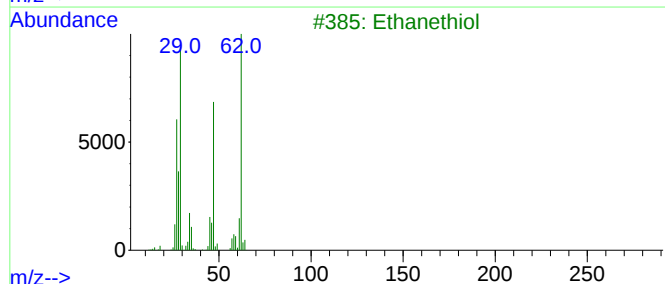
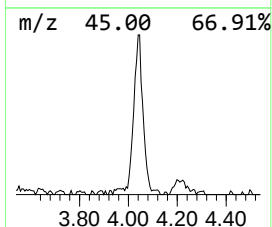
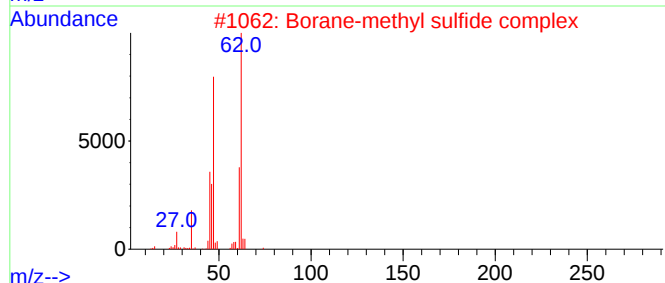
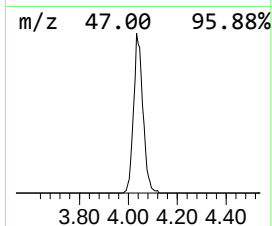
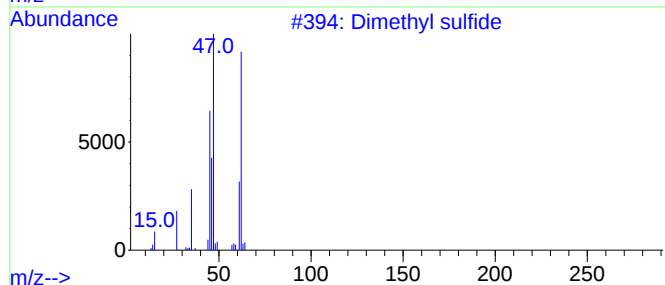
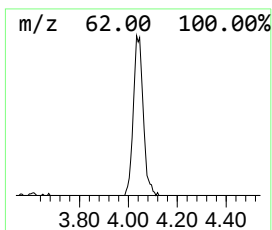
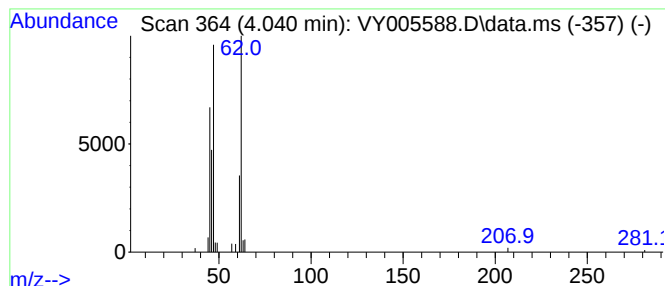
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y080221S.M
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TIC Integration Parameters: LSCINT.P

Peak Number 1 Dimethyl sulfide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.040	5.10 ug/l	66116	Pentafluorobenzene	7.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl sulfide	62	C2H6S	000075-18-3	94
2			Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	83
3			Ethanethiol	62	C2H6S	000075-08-1	72
4			Acetic acid, mercapto-, methyl e...	106	C3H6O2S	002365-48-2	22
5			Acetic acid, 2,2'-thiobis-	150	C4H6O4S	000123-93-3	12



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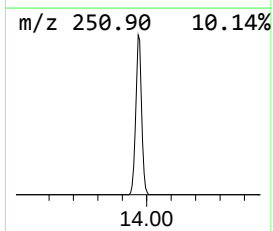
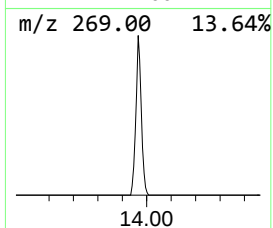
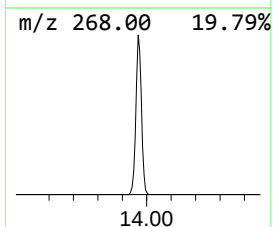
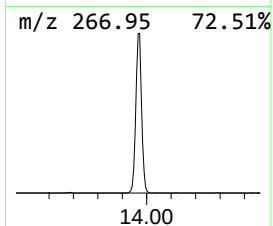
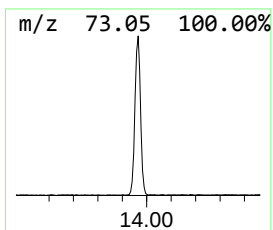
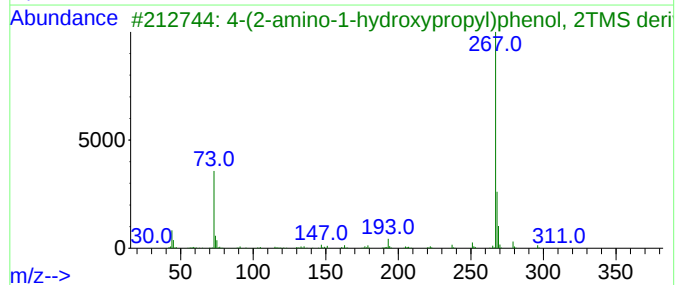
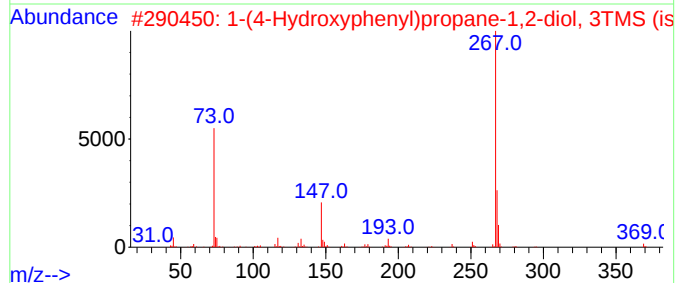
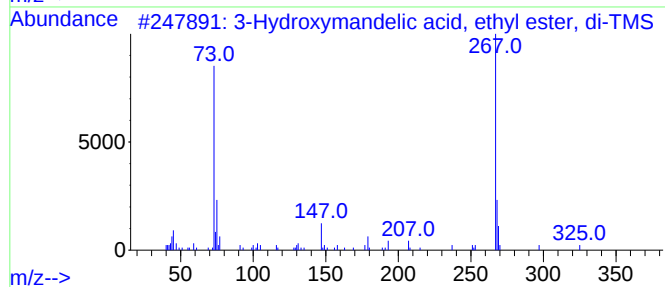
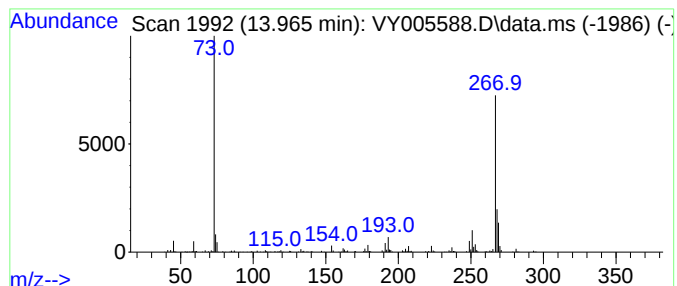
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Peak Number 3 3-Hydroxymandelic acid, eth... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.965	10.18 ug/l	251573	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hydroxymandelic acid, ethyl es...	340	C16H28O4Si2	1000071-88-9	64
2			1-(4-Hydroxyphenyl)propane-1,2-d...	384	C18H36O3Si3	1000495-85-7	64
3			4-(2-amino-1-hydroxypropyl)pheno...	311	C15H29NO2Si2	1000478-98-6	64
4			p-Trimethylsilyloxyphenyl-bis(tr...	370	C17H34O3Si3	1000079-08-1	59
5			2,5-Dihydroxybenzaldehyde, 2TMS ...	282	C13H22O3Si2	056114-69-3	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Dimethyl sulfide	4.040	5.1	ug/l	66116	1	7.795	647943	50.0
3-Hydroxymandel...	13.965	10.2	ug/l	251573	4	13.428	1235510	50.0