

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY092921\
 Data File : VY006215.D
 Acq On : 29 Sep 2021 16:05
 Operator : SY/MD
 Sample : M3987-01
 Misc : 4.97G/5ML/MSVOA_Y/SOIL
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 SS02-NA

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\82Y092821S.M
 Title : SW846 8260

Signal : TIC: VY006215.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.064	39	40	45	rVB3	690	834	1.64%	0.306%
2	2.345	84	86	87	rVB2	1031	580	1.14%	0.213%
3	2.558	119	121	123	rVB3	654	523	1.03%	0.192%
4	2.619	129	131	136	rVB3	928	1148	2.26%	0.421%
5	2.936	181	183	186	rVB2	548	527	1.04%	0.193%
6	3.271	234	238	239	rBV3	479	577	1.13%	0.211%
7	3.375	251	255	264	rVB4	1114	3177	6.24%	1.164%
8	3.491	271	274	279	rVB3	286	557	1.09%	0.204%
9	3.948	341	349	351	rBV3	1051	2030	3.99%	0.744%
10	4.040	358	364	371	rBV7	1431	3883	7.63%	1.423%
11	4.704	469	473	474	rBV2	682	851	1.67%	0.312%
12	4.722	474	476	483	rVV3	840	1854	3.64%	0.680%
13	5.765	640	647	651	rVB6	566	1588	3.12%	0.582%
14	7.722	960	968	974	rBV3	5201	11570	22.74%	4.241%
15	7.795	974	980	989	rVB	14196	31428	61.76%	11.519%
16	8.149	1031	1038	1047	rBV2	7125	16095	31.63%	5.899%
17	8.697	1117	1128	1135	rBV	19208	38016	74.71%	13.933%
18	9.984	1334	1339	1346	rVB2	4913	8691	17.08%	3.185%
19	10.185	1363	1372	1381	rVB	29755	50888	100.00%	18.651%
20	11.496	1581	1587	1594	rBV	23563	38041	74.75%	13.942%
21	12.337	1722	1725	1731	rVB3	1117	1548	3.04%	0.567%
22	12.483	1742	1749	1757	rVB2	15800	24581	48.30%	9.009%
23	13.428	1898	1904	1910	rVB2	16856	25818	50.73%	9.463%
24	14.081	2008	2011	2016	rVB2	346	589	1.16%	0.216%
25	14.166	2022	2025	2028	rBV	325	530	1.04%	0.194%
26	14.818	2128	2132	2133	rBV2	498	565	1.11%	0.207%
27	15.318	2211	2214	2216	rVB3	541	642	1.26%	0.235%
28	15.373	2220	2223	2225	rBV3	515	716	1.41%	0.262%
29	15.550	2251	2252	2256	rBV5	532	589	1.16%	0.216%
30	15.641	2265	2267	2271	rVB2	500	680	1.34%	0.249%
31	15.708	2274	2278	2281	rBV3	596	1088	2.14%	0.399%
32	15.928	2311	2314	2316	rBV4	454	545	1.07%	0.200%
33	16.251	2365	2367	2369	rBV2	799	784	1.54%	0.287%
34	16.525	2407	2412	2413	rBV3	596	767	1.51%	0.281%
35	16.641	2428	2431	2433	rVB2	570	545	1.07%	0.200%

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SS02-NA

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\82Y092821S.M
Title : SW846 8260

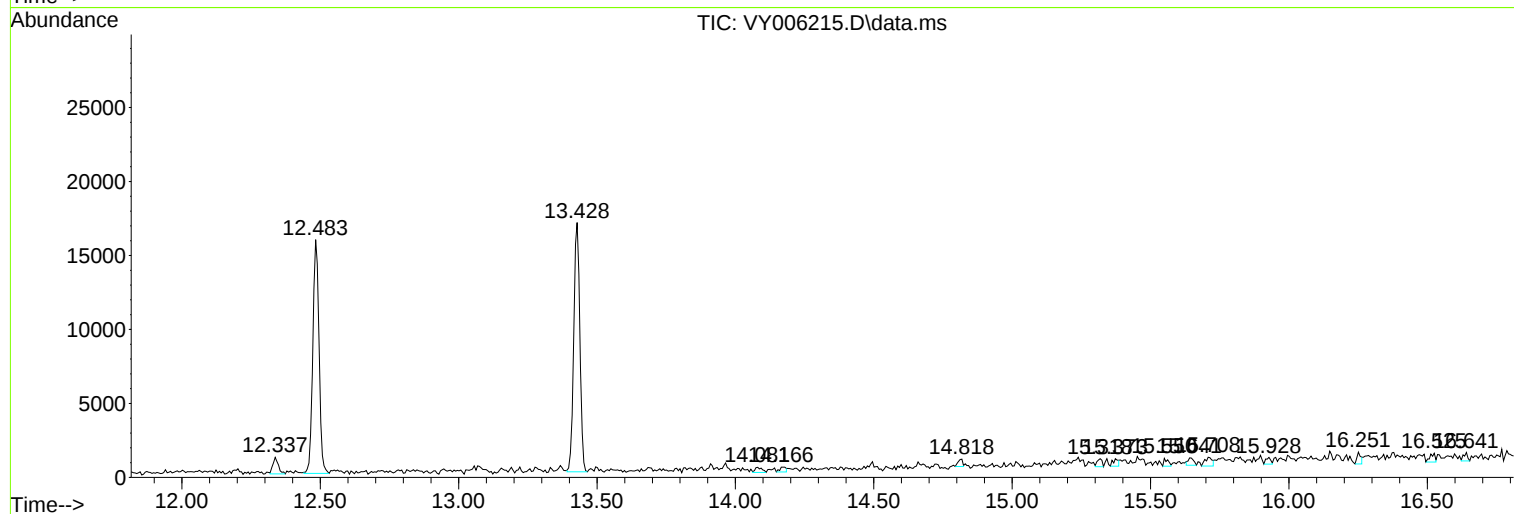
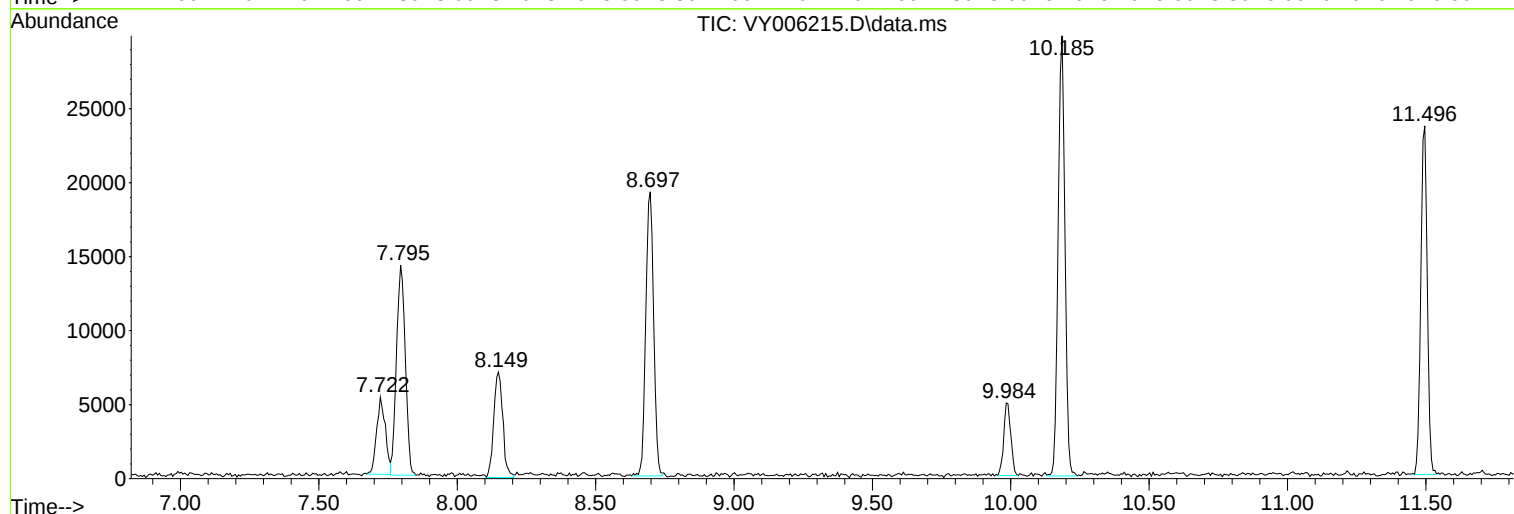
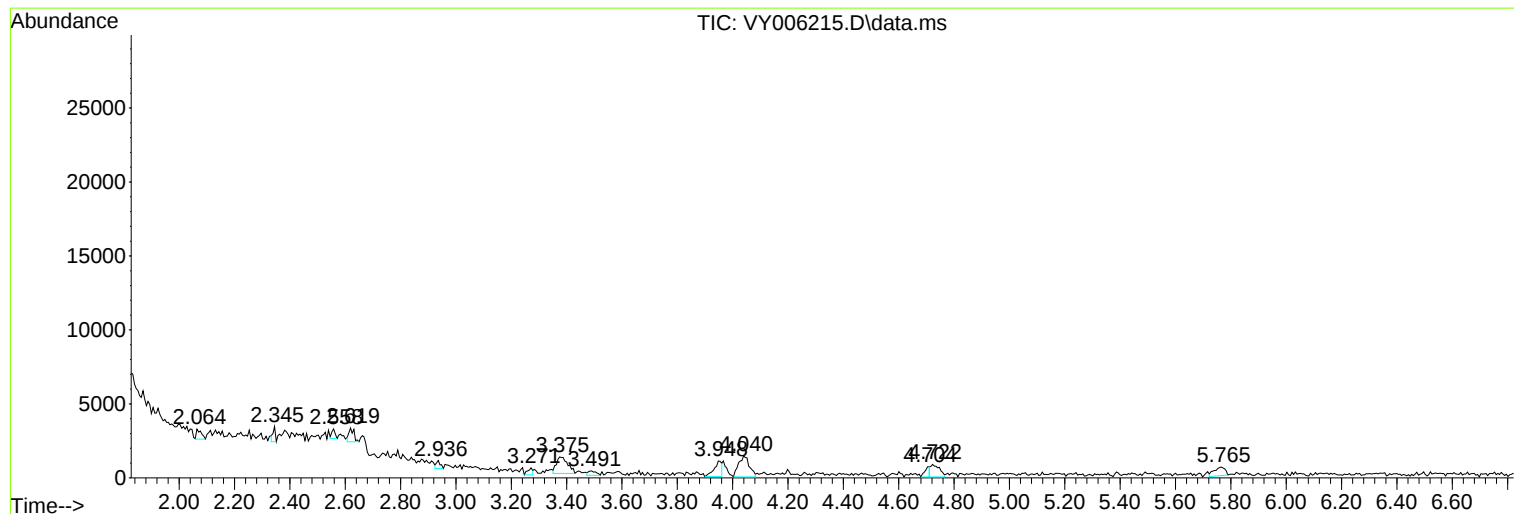
Sum of corrected areas: 272845

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y092821S.M
Quant Title : SW846 8260

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



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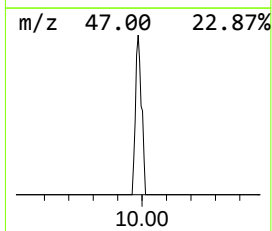
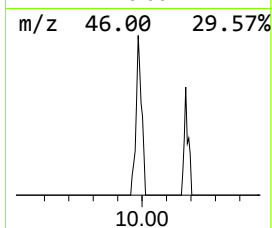
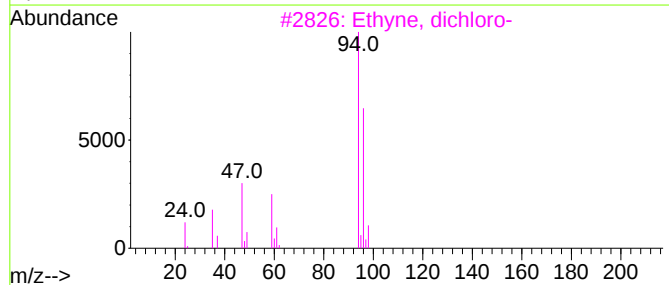
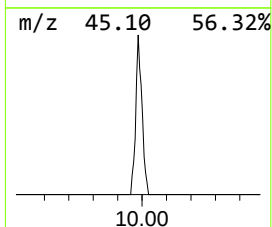
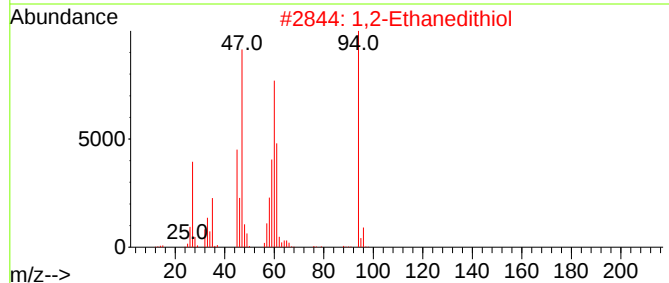
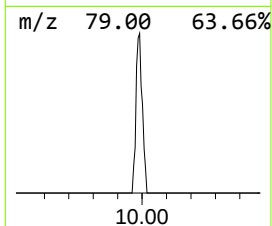
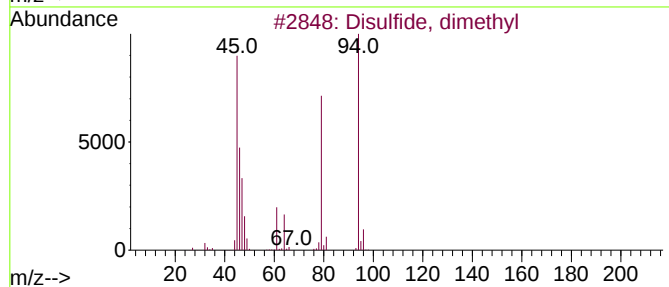
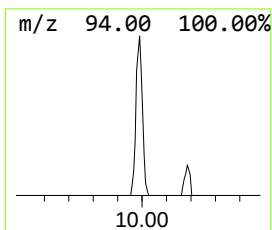
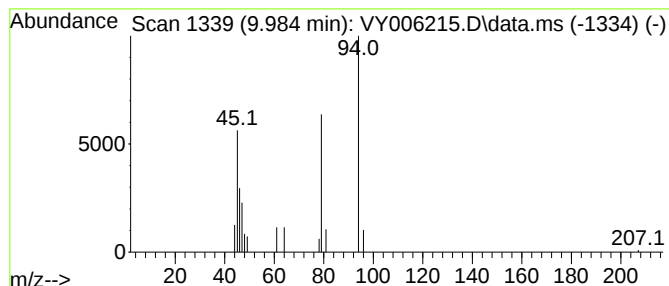
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y092821S.M
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 3 Disulfide, dimethyl Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.984	11.43 ug/l	8691	1,4-Difluorobenzene	8.697

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Disulfide, dimethyl	94	C2H6S2	000624-92-0	91
2			1,2-Ethanedithiol	94	C2H6S2	000540-63-6	46
3			Ethyne, dichloro-	94	C2Cl2	007572-29-4	25
4			S-(2,2,2-Trifluoroethyl) methane...	194	C3H5F3O2S2	069466-44-0	25
5			Isothiourea, 2-methylthiomethyl-	136	C3H8N2S2	090484-97-2	12



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Disulfide, dime...	9.984	11.4	ug/l	8691	2	8.697	38016	50.0