

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX102220\
 Data File : VX019064.D
 Acq On : 23 Oct 2020 06:11
 Operator : JC/SP
 Sample : L4489-01
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 55 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 201021075-01-VOA

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X102120W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.373	44	47	55	rVB	14931	18291	1.21%	0.174%
2	1.581	76	81	87	rBV3	9900	17242	1.14%	0.164%
3	2.166	172	177	187	rBV	34618	50533	3.33%	0.481%
4	2.459	214	225	236	rVB2	154732	300257	19.80%	2.861%
5	3.007	306	315	328	rBV	70137	160263	10.57%	1.527%
6	4.641	567	583	599	rBV	114065	385289	25.41%	3.671%
7	5.086	645	656	673	rBV	120180	369108	24.35%	3.517%
8	5.464	707	718	732	rBV	169196	488015	32.19%	4.649%
9	5.629	732	745	764	rVB2	271868	785125	51.78%	7.480%
10	6.031	800	811	821	rBV	175096	465933	30.73%	4.439%
11	6.830	931	942	953	rBV	441583	1039390	68.55%	9.902%
12	7.720	1081	1088	1100	rBV	10691	22691	1.50%	0.216%
13	8.458	1203	1209	1220	rBV	83573	153119	10.10%	1.459%
14	8.695	1240	1248	1255	rBV	949365	1480725	97.66%	14.107%
15	8.762	1255	1259	1268	rVB3	18368	36420	2.40%	0.347%
16	9.421	1358	1367	1373	rBV	12975	20150	1.33%	0.192%
17	9.531	1380	1385	1391	rBV	16904	24790	1.64%	0.236%
18	10.097	1465	1478	1490	rBV	946217	1407899	92.86%	13.413%
19	10.238	1496	1501	1511	rBV2	23844	39618	2.61%	0.377%
20	10.341	1511	1518	1524	rVB	60284	86135	5.68%	0.821%
21	10.683	1569	1574	1581	rVB	38312	51455	3.39%	0.490%
22	11.000	1620	1626	1632	rBV	15092	21428	1.41%	0.204%
23	11.122	1640	1646	1652	rBV	824365	1037169	68.41%	9.881%
24	11.652	1729	1733	1738	rBV	18764	25084	1.65%	0.239%
25	11.792	1751	1756	1760	rVB	24491	31079	2.05%	0.296%
26	11.926	1770	1778	1785	rVB	32194	46049	3.04%	0.439%
27	12.061	1794	1800	1808	rBV	1146587	1516153	100.00%	14.445%
28	12.128	1808	1811	1816	rVB	15136	20287	1.34%	0.193%
29	12.280	1831	1836	1841	rBV	40432	55627	3.67%	0.530%
30	12.371	1845	1851	1859	rVB4	10803	22979	1.52%	0.219%
31	12.804	1919	1922	1927	rVB	17220	21558	1.42%	0.205%
32	13.329	2003	2008	2013	rBV2	16696	23294	1.54%	0.222%
33	13.512	2033	2038	2041	rBV3	20914	29487	1.94%	0.281%
34	13.548	2041	2044	2048	rVB	19797	24175	1.59%	0.230%

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Title : SW846 8260

35	13.627	2052	2057	2062	rBV2	33314	50091	3.30%	0.477%
36	13.816	2083	2088	2094	rVB	69001	90181	5.95%	0.859%
37	13.889	2094	2100	2108	rVB3	8223	20285	1.34%	0.193%
38	13.969	2108	2113	2120	rBV7	8020	18598	1.23%	0.177%
39	14.682	2225	2230	2232	rBV2	13180	21060	1.39%	0.201%
40	14.822	2248	2253	2260	rVB2	14179	19276	1.27%	0.184%

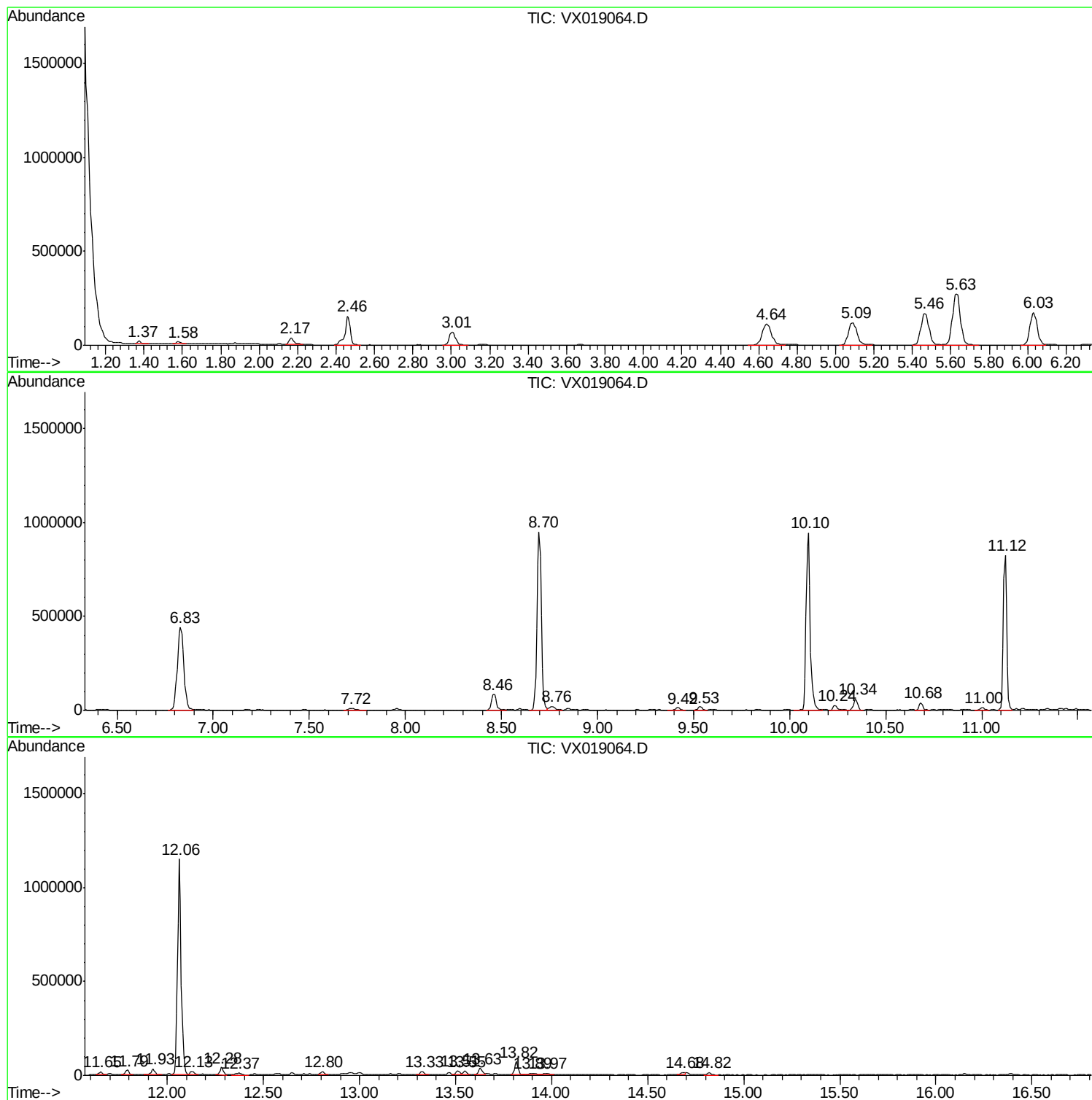
Sum of corrected areas: 10496308

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X102120W.M
Quant Title : SW846 8260

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



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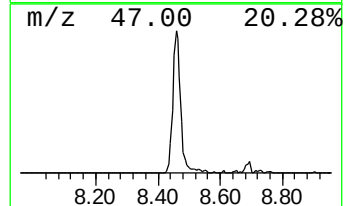
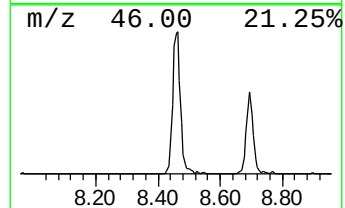
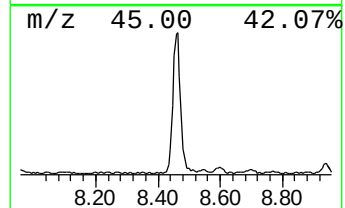
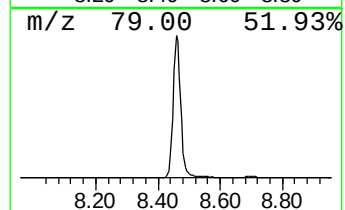
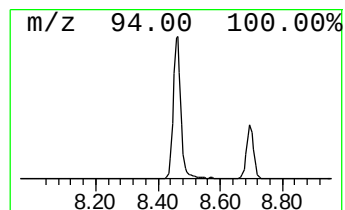
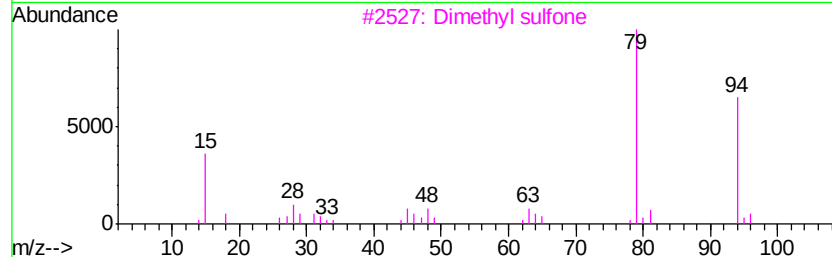
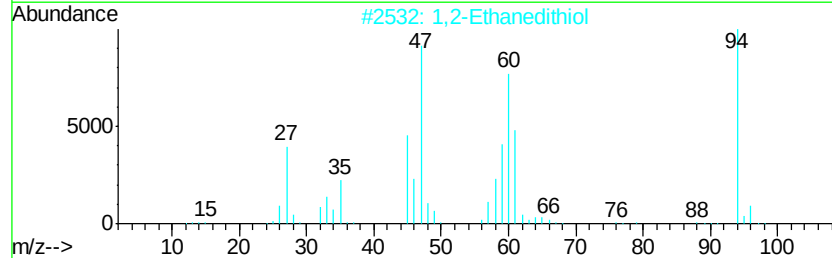
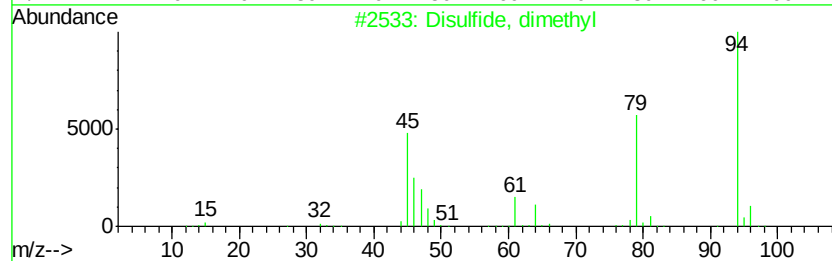
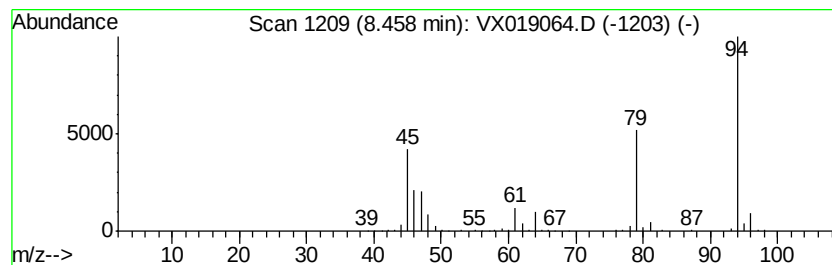
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Disulfide, dimethyl Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.46	7.37 ug/l	153119	1,4-Difluorobenzene	6.83	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Disulfide, dimethyl	94	C2H6S2	000624-92-0	96
2	1,2-Ethanedithiol	94	C2H6S2	000540-63-6	52
3	Dimethyl sulfone	94	C2H6O2S	000067-71-0	46
4	Methanesulfonyl chloride	114	CH3ClO2S	000124-63-0	7
5	Pyrazine, methyl-	94	C5H6N2	000109-08-0	5



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Disulfide, dimethyl	8.46	7.4	ug/l	153119	2	6.83	1039390	50.0