

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW042224\
 Data File : VW028506.D
 Acq On : 22 Apr 2024 13:28
 Operator : SY/MD
 Sample : P2203-13
 Misc : 3.14g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 E1CY7

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % 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_W\Method\SFAMWLM040824SMA.M
 Title : SFAM01.0

Signal : TIC: VW028506.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.003	17	19	21	rVB3	1343	1153	0.06%	0.009%
2	2.149	39	43	45	rBV5	1594	2635	0.15%	0.021%
3	2.204	49	52	53	rBV3	2397	2329	0.13%	0.018%
4	2.253	58	60	63	rVV4	1707	1528	0.09%	0.012%
5	2.363	71	78	89	rBV	122253	264149	14.85%	2.095%
6	2.899	159	166	180	rVB	85501	240425	13.52%	1.907%
7	3.198	213	215	219	rBV4	876	1433	0.08%	0.011%
8	3.247	222	223	227	rVB4	1549	1122	0.06%	0.009%
9	3.283	227	229	231	rBV3	1108	1005	0.06%	0.008%
10	3.344	237	239	241	rVB3	1176	935	0.05%	0.007%
11	3.381	241	245	246	rBV4	792	922	0.05%	0.007%
12	3.503	262	265	267	rVV4	1384	1935	0.11%	0.015%
13	3.539	269	271	272	rVV2	1348	1106	0.06%	0.009%
14	3.570	275	276	279	rVV3	1158	1080	0.06%	0.009%
15	3.637	284	287	288	rBV3	972	947	0.05%	0.008%
16	3.753	303	306	308	rBV4	1418	1556	0.09%	0.012%
17	3.826	315	318	320	rBV4	1393	1375	0.08%	0.011%
18	4.021	338	350	366	rBV	194892	592926	33.34%	4.704%
19	4.192	377	378	381	rBV3	1430	1059	0.06%	0.008%
20	4.222	381	383	385	rBV3	1015	931	0.05%	0.007%
21	4.332	397	401	402	rBV4	851	950	0.05%	0.008%
22	4.533	432	434	437	rVB4	975	960	0.05%	0.008%
23	4.917	486	497	510	rBV	26170	91895	5.17%	0.729%
24	5.063	518	521	522	rBV2	1162	966	0.05%	0.008%
25	5.137	529	533	534	rBV4	1476	2037	0.11%	0.016%
26	5.155	534	536	538	rVV3	1101	1329	0.07%	0.011%
27	5.222	545	547	549	rVB3	1452	1299	0.07%	0.010%
28	5.252	549	552	553	rBV3	1039	974	0.05%	0.008%
29	5.326	559	564	565	rBV5	969	1751	0.10%	0.014%
30	5.350	565	568	570	rVB4	774	927	0.05%	0.007%
31	5.429	579	581	585	rBV5	1049	1032	0.06%	0.008%
32	5.807	639	643	645	rBV5	791	996	0.06%	0.008%
33	5.874	652	654	658	rBV5	890	1543	0.09%	0.012%
34	5.941	658	665	667	rBV8	5693	11999	0.67%	0.095%
35	6.008	675	676	679	rVB3	1044	968	0.05%	0.008%
36	6.045	679	682	684	rBV4	1148	1553	0.09%	0.012%

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 Title : SFAM01.0

37	6.167	699	702	704	rBV3	1308	1304	0.07%	0.010%
38	6.252	713	716	719	rVB5	963	998	0.06%	0.008%
39	6.283	719	721	725	rVB5	1251	1445	0.08%	0.011%
40	6.325	725	728	731	rBV5	787	1396	0.08%	0.011%
41	6.453	744	749	752	rVB7	1581	2282	0.13%	0.018%
42	6.691	786	788	791	rBV4	785	1025	0.06%	0.008%
43	6.898	820	822	826	rBV4	969	1095	0.06%	0.009%
44	6.966	831	833	834	rBV2	988	1020	0.06%	0.008%
45	6.984	834	836	841	rVB6	954	1211	0.07%	0.010%
46	7.075	843	851	869	rBV2	44173	151544	8.52%	1.202%
47	7.362	894	898	900	rBV4	983	1357	0.08%	0.011%
48	7.447	903	912	922	rVV3	16686	45223	2.54%	0.359%
49	7.648	935	945	959	rBV	297672	774135	43.53%	6.141%
50	7.910	987	988	991	rBV3	938	980	0.06%	0.008%
51	7.947	991	994	996	rBV3	1028	1000	0.06%	0.008%
52	8.014	1004	1005	1011	rBV6	1277	1775	0.10%	0.014%
53	8.118	1018	1022	1025	rVB6	858	924	0.05%	0.007%
54	8.276	1037	1048	1065	rBV2	616038	1778533	100.00%	14.109%
55	8.691	1112	1116	1119	rBV6	1060	1401	0.08%	0.011%
56	8.758	1125	1127	1130	rBV4	965	961	0.05%	0.008%
57	8.843	1130	1141	1151	rBV	666608	1338746	75.27%	10.620%
58	8.941	1156	1157	1159	rVV2	1429	1401	0.08%	0.011%
59	9.075	1172	1179	1189	rVV	82069	162926	9.16%	1.292%
60	9.270	1203	1211	1222	rVV	425498	871948	49.03%	6.917%
61	9.447	1239	1240	1242	rBV2	1474	1203	0.07%	0.010%
62	9.514	1248	1251	1252	rBV3	1327	1223	0.07%	0.010%
63	9.666	1272	1276	1278	rBV5	1563	2217	0.12%	0.018%
64	9.752	1284	1290	1291	rBV6	1090	1992	0.11%	0.016%
65	9.892	1310	1313	1318	rVB6	1516	2105	0.12%	0.017%
66	10.032	1327	1336	1344	rBV	189648	347004	19.51%	2.753%
67	10.136	1350	1353	1354	rVB3	1236	1019	0.06%	0.008%
68	10.319	1375	1383	1391	rBV	810499	1441463	81.05%	11.435%
69	10.386	1391	1394	1407	rVB2	13352	30312	1.70%	0.240%
70	10.575	1417	1425	1436	rBV	105827	182731	10.27%	1.450%
71	10.697	1442	1445	1455	rVB7	4658	10427	0.59%	0.083%
72	10.770	1455	1457	1458	rBV2	1606	1364	0.08%	0.011%
73	10.855	1467	1471	1476	rBV8	2111	3964	0.22%	0.031%
74	10.922	1476	1482	1494	rBV	161181	282156	15.86%	2.238%
75	11.373	1553	1556	1559	rBV4	1228	2111	0.12%	0.017%
76	11.629	1589	1598	1608	rBV	824913	1376794	77.41%	10.922%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM040824SMA.M
 Title : SFAM01.0

77	11.709	1608	1611	1612	rVV3	3134	3575	0.20%	0.028%
78	11.727	1612	1614	1618	rVV5	3968	4830	0.27%	0.038%
79	11.794	1621	1625	1626	rBV4	1060	1160	0.07%	0.009%
80	11.837	1628	1632	1635	rBV6	2497	4285	0.24%	0.034%
81	12.166	1682	1686	1687	rBV4	1757	2414	0.14%	0.019%
82	12.251	1695	1700	1701	rBV5	1547	1887	0.11%	0.015%
83	12.306	1707	1709	1710	rBV2	1311	1293	0.07%	0.010%
84	12.349	1713	1716	1717	rBV3	1315	1422	0.08%	0.011%
85	12.513	1741	1743	1746	rBV4	1115	1435	0.08%	0.011%
86	12.586	1749	1755	1764	rBV3	16063	36553	2.06%	0.290%
87	12.690	1764	1772	1778	rVV	232903	376654	21.18%	2.988%
88	12.751	1779	1782	1791	rVB3	5950	12610	0.71%	0.100%
89	12.836	1794	1796	1797	rBV2	1467	1281	0.07%	0.010%
90	12.958	1810	1816	1822	rBV10	4427	8176	0.46%	0.065%
91	13.117	1838	1842	1845	rBV5	5591	8051	0.45%	0.064%
92	13.190	1850	1854	1859	rVB	27281	40780	2.29%	0.323%
93	13.300	1866	1872	1879	rVB	20801	35155	1.98%	0.279%
94	13.403	1881	1889	1896	rBV	39058	76035	4.28%	0.603%
95	13.556	1907	1914	1919	rBV	569546	934843	52.56%	7.416%
96	13.763	1943	1948	1955	rVB2	14775	26858	1.51%	0.213%
97	13.848	1955	1962	1972	rBV2	557027	917342	51.58%	7.277%
98	14.062	1993	1997	2002	rVB2	6031	9375	0.53%	0.074%
99	14.501	2063	2069	2070	rBV5	3800	6622	0.37%	0.053%
100	15.427	2218	2221	2227	rVB3	12779	18824	1.06%	0.149%

Sum of corrected areas: 12605905

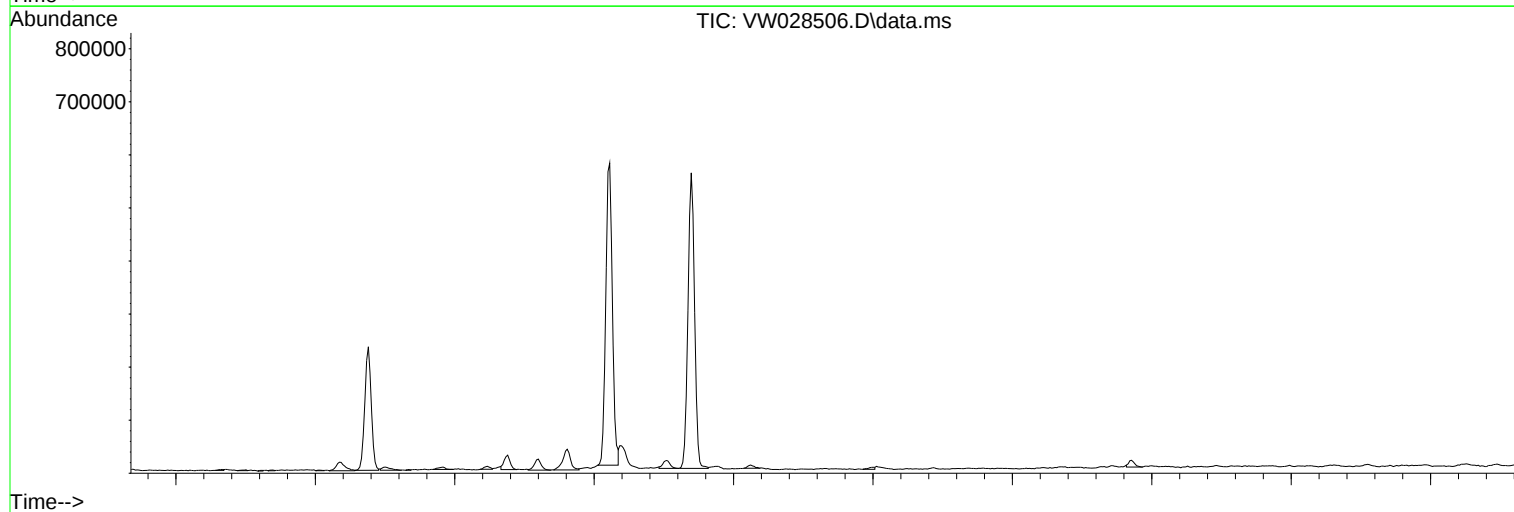
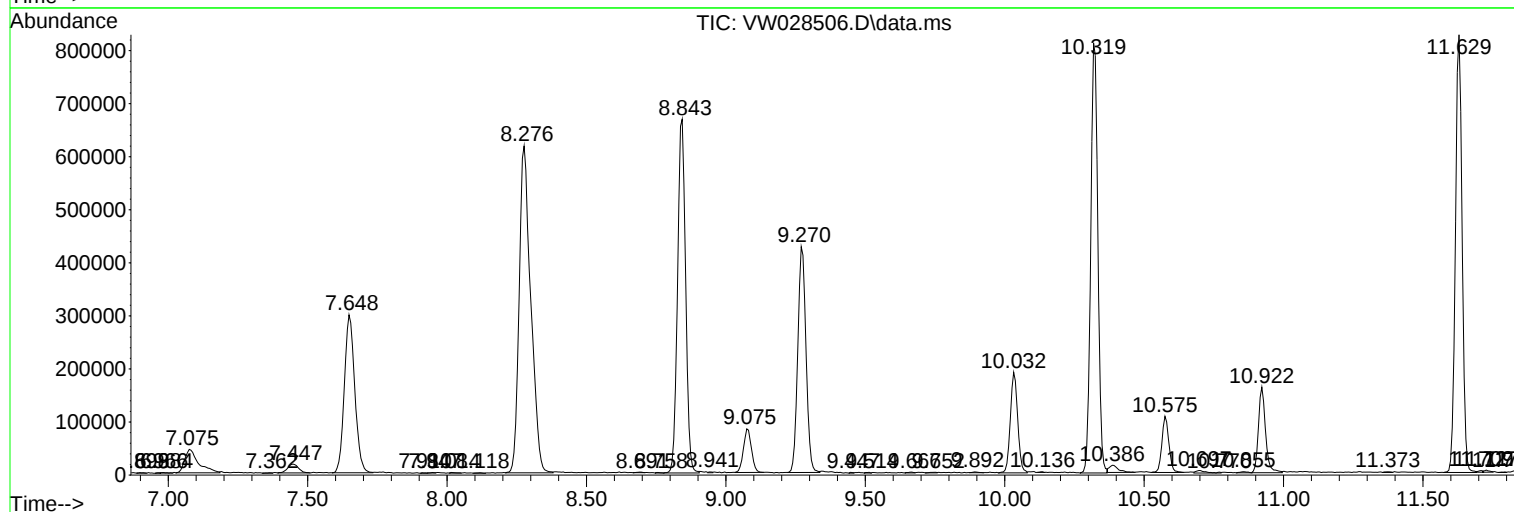
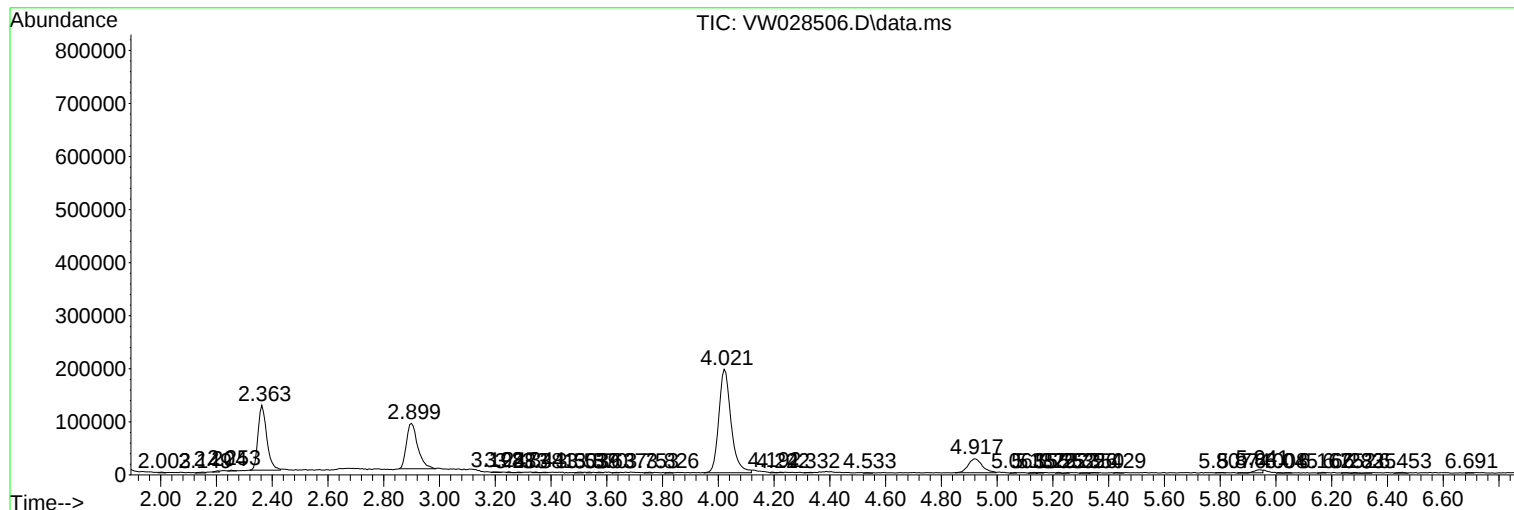
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM040824SMA.M
Quant Title : SFAM01.0

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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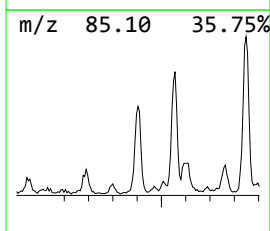
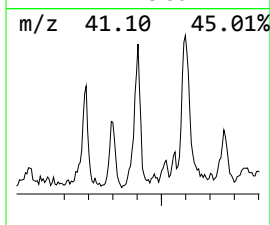
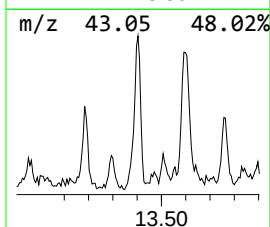
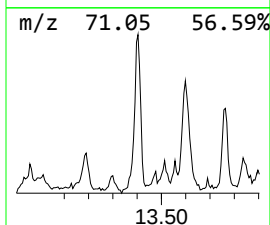
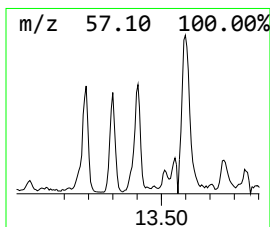
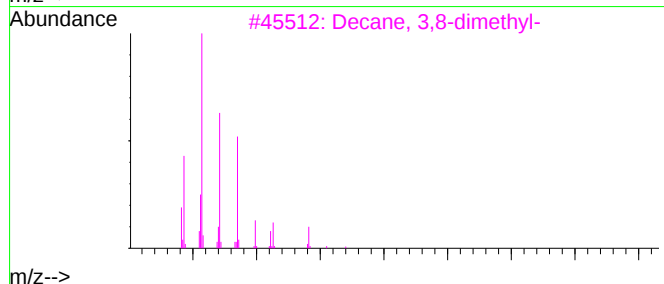
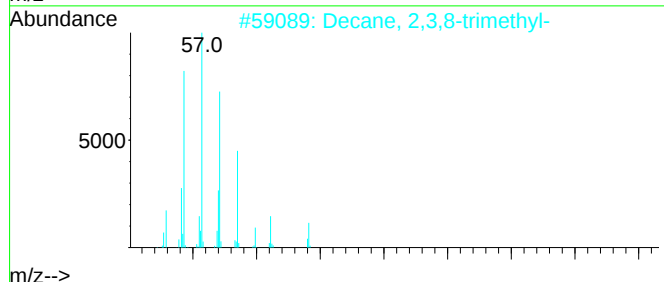
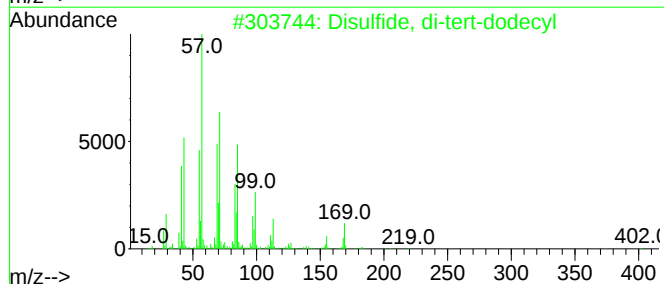
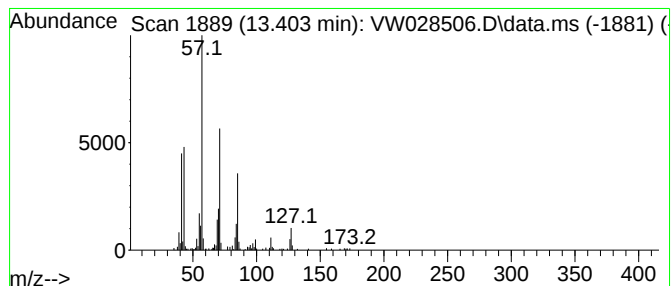
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM040824SMA.M
Quant Title : SFAM01.0

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 Disulfide, di-tert-dodecyl Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.403	2.03 ug/L	76035	1,4-Dichlorobenzene-d4	13.556	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	64
2	Decane, 2,3,8-trimethyl-	184	C13H28	062238-14-6	59
3	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	58
4	Sulfurous acid, 2-pentyl undecyl...	306	C16H34O3S	1000309-16-0	50
5	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Disulfide, di-t...	13.403	2.0	ug/L	76035	3	13.556	934843	25.0