

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW071624\
 Data File : VW029590.D
 Acq On : 16 Jul 2024 15:15
 Operator : SY/MD
 Sample : P3263-01
 Misc : 5.25g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 A4BA0

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % 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_W\Method\SFAMWLM070824SMA.M

Title : SFAM01.0

Signal : TIC: VW029590.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.149	41	43	45	rBV2	961	1148	0.09%	0.011%
2	2.216	50	54	57	rBV2	3352	5531	0.41%	0.053%
3	2.363	72	78	94	rBV	45923	138854	10.36%	1.335%
4	2.893	158	165	180	rBV2	44770	136805	10.21%	1.316%
5	3.234	219	221	222	rBV2	1067	881	0.07%	0.008%
6	3.442	251	255	257	rBV3	695	1014	0.08%	0.010%
7	3.478	259	261	264	rBV3	914	989	0.07%	0.010%
8	3.734	299	303	305	rBV5	705	1144	0.09%	0.011%
9	4.015	337	349	366	rBV2	104564	416909	31.11%	4.010%
10	4.375	402	408	409	rBV5	1294	2118	0.16%	0.020%
11	4.917	481	497	526	rBV2	41440	200569	14.96%	1.929%
12	5.100	526	527	531	rVV4	1075	790	0.06%	0.008%
13	5.429	571	581	590	rVV7	5522	18628	1.39%	0.179%
14	5.557	599	602	608	rBV6	741	1261	0.09%	0.012%
15	5.807	641	643	646	rVB3	874	957	0.07%	0.009%
16	5.935	659	664	670	rBV6	2176	5113	0.38%	0.049%
17	6.149	696	699	701	rBV3	651	843	0.06%	0.008%
18	6.173	701	703	704	rBV2	898	824	0.06%	0.008%
19	6.197	704	707	708	rBV3	2134	2059	0.15%	0.020%
20	6.368	732	735	739	rVB4	602	923	0.07%	0.009%
21	6.594	770	772	775	rVB3	825	1024	0.08%	0.010%
22	6.734	792	795	797	rBV3	636	770	0.06%	0.007%
23	6.886	814	820	822	rBV4	681	1143	0.09%	0.011%
24	7.075	842	851	860	rBV	31387	97673	7.29%	0.939%
25	7.404	903	905	908	rBV2	565	734	0.05%	0.007%
26	7.502	912	921	922	rBV5	3244	4926	0.37%	0.047%
27	7.642	934	944	958	rBV	225482	564109	42.09%	5.426%
28	7.862	973	980	988	rBV4	3934	10932	0.82%	0.105%
29	7.953	988	995	1005	rVV6	5895	16614	1.24%	0.160%
30	8.063	1006	1013	1021	rVB4	3724	10264	0.77%	0.099%
31	8.270	1037	1047	1063	rVV2	439405	1300892	97.06%	12.512%
32	8.398	1063	1068	1077	rVB3	3844	9663	0.72%	0.093%
33	8.538	1089	1091	1094	rVB4	928	749	0.06%	0.007%
34	8.605	1098	1102	1103	rBV2	600	720	0.05%	0.007%
35	8.837	1131	1140	1152	rBV	596463	1156081	86.26%	11.119%
36	9.087	1172	1181	1190	rBV5	10133	22930	1.71%	0.221%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM070824SMA.M
 Title : SFAM01.0

37	9.215	1199	1202	1203	rBV2	916	998	0.07%	0.010%
38	9.270	1203	1211	1218	rBV	311324	629471	46.97%	6.054%
39	9.642	1265	1272	1281	rBV4	5064	13366	1.00%	0.129%
40	9.825	1299	1302	1304	rVB2	582	748	0.06%	0.007%
41	9.886	1307	1312	1321	rVB6	1341	3778	0.28%	0.036%
42	10.032	1321	1336	1348	rBV	151166	292668	21.84%	2.815%
43	10.203	1360	1364	1371	rBV2	3282	7195	0.54%	0.069%
44	10.319	1375	1383	1390	rBV	583242	1012712	75.56%	9.740%
45	10.386	1390	1394	1401	rVB	12939	24895	1.86%	0.239%
46	10.501	1410	1413	1416	rVB3	718	1064	0.08%	0.010%
47	10.575	1418	1425	1437	rBV	94913	173227	12.92%	1.666%
48	10.703	1439	1446	1451	rVB2	5652	11186	0.83%	0.108%
49	10.788	1451	1460	1464	rBV7	6126	12864	0.96%	0.124%
50	10.855	1464	1471	1476	rBV	25482	47177	3.52%	0.454%
51	10.922	1476	1482	1497	rVB	126240	228925	17.08%	2.202%
52	11.123	1511	1515	1520	rVV4	3009	4941	0.37%	0.048%
53	11.172	1520	1523	1528	rVB5	2478	3371	0.25%	0.032%
54	11.233	1529	1533	1538	rVB3	1928	3212	0.24%	0.031%
55	11.337	1545	1550	1556	rBV8	1840	3176	0.24%	0.031%
56	11.410	1556	1562	1569	rVV8	2041	4754	0.35%	0.046%
57	11.629	1587	1598	1607	rBV	789477	1340282	100.00%	12.891%
58	11.727	1610	1614	1621	rVB	16634	28919	2.16%	0.278%
59	11.837	1625	1632	1636	rBV	12019	24167	1.80%	0.232%
60	12.062	1665	1669	1672	rBV4	2340	3232	0.24%	0.031%
61	12.093	1672	1674	1680	rVV7	1135	2041	0.15%	0.020%
62	12.166	1680	1686	1695	rVB3	17123	37612	2.81%	0.362%
63	12.343	1710	1715	1719	rBV6	2313	5064	0.38%	0.049%
64	12.458	1729	1734	1740	rVV	14801	24365	1.82%	0.234%
65	12.586	1749	1755	1762	rBV2	7991	18112	1.35%	0.174%
66	12.690	1764	1772	1779	rBV	197254	330012	24.62%	3.174%
67	12.763	1779	1784	1792	rVB7	5837	14002	1.04%	0.135%
68	12.843	1793	1797	1798	rVB4	726	770	0.06%	0.007%
69	12.885	1800	1804	1807	rBV5	1275	1759	0.13%	0.017%
70	12.940	1807	1813	1821	rBV3	12456	27154	2.03%	0.261%
71	13.007	1821	1824	1827	rBV5	1374	1956	0.15%	0.019%
72	13.086	1831	1837	1839	rBV7	1096	1716	0.13%	0.017%
73	13.123	1840	1843	1845	rBV4	1088	1267	0.09%	0.012%
74	13.184	1845	1853	1858	rBV	16859	28336	2.11%	0.273%
75	13.245	1858	1863	1867	rBV	9798	14732	1.10%	0.142%
76	13.294	1867	1871	1877	rVB	8811	14638	1.09%	0.141%

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 Title : SFAM01.0

77	13.403	1881	1889	1894	rBV	28417	53153	3.97%	0.511%
78	13.501	1896	1905	1907	rBV5	12062	27674	2.06%	0.266%
79	13.550	1907	1913	1919	rBV	623996	1026525	76.59%	9.873%
80	13.757	1941	1947	1955	rVB	16312	31818	2.37%	0.306%
81	13.848	1955	1962	1969	rBV	388062	650006	48.50%	6.252%
82	14.214	2016	2022	2023	rBV5	909	1672	0.12%	0.016%
83	14.324	2036	2040	2046	rVB6	2930	5686	0.42%	0.055%
84	14.415	2051	2055	2056	rBV4	780	1141	0.09%	0.011%
85	14.482	2060	2066	2067	rVV5	2004	2916	0.22%	0.028%
86	14.513	2069	2071	2080	rVV5	3745	6805	0.51%	0.065%
87	14.623	2083	2089	2095	rVB2	8545	13684	1.02%	0.132%
88	14.684	2095	2099	2102	rBV5	989	1826	0.14%	0.018%
89	14.720	2102	2105	2108	rVB4	2061	2741	0.20%	0.026%
90	15.129	2166	2172	2179	rVV3	5477	9949	0.74%	0.096%
91	15.196	2179	2183	2188	rVV4	1584	3080	0.23%	0.030%
92	15.245	2188	2191	2196	rVB6	1591	2573	0.19%	0.025%
93	15.324	2201	2204	2205	rBV3	615	766	0.06%	0.007%
94	15.366	2205	2211	2221	rVB	3366	8011	0.60%	0.077%
95	15.476	2227	2229	2232	rBV4	885	985	0.07%	0.009%
96	15.543	2236	2240	2245	rVV6	3970	6662	0.50%	0.064%
97	15.616	2251	2252	2255	rBV3	687	753	0.06%	0.007%
98	16.464	2388	2391	2393	rBV4	687	831	0.06%	0.008%
99	16.598	2411	2413	2415	rBV3	797	757	0.06%	0.007%
100	16.659	2420	2423	2426	rBV5	580	765	0.06%	0.007%

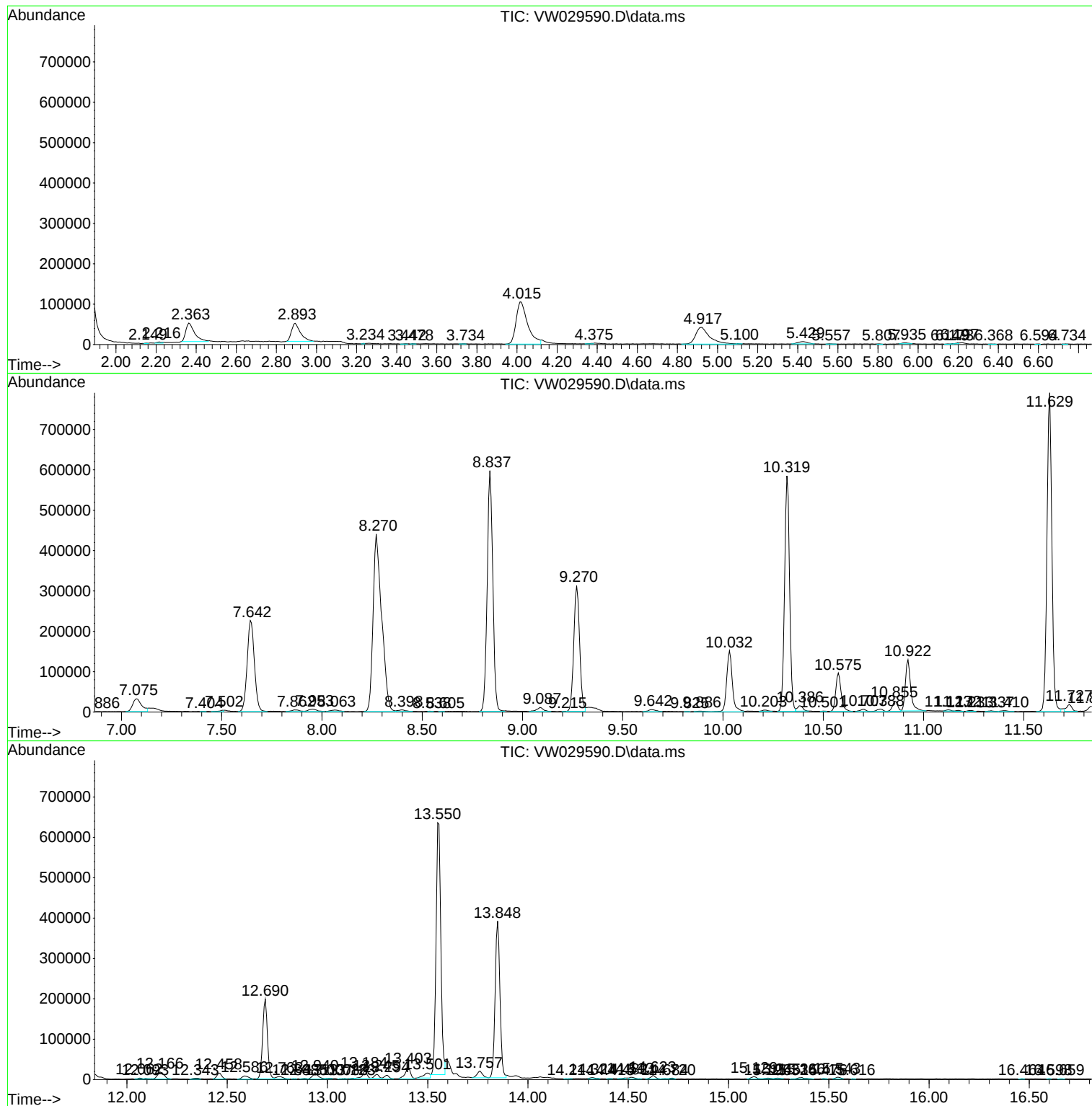
Sum of corrected areas: 10397227

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM070824SMA.M
Quant Title : SFAM01.0

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



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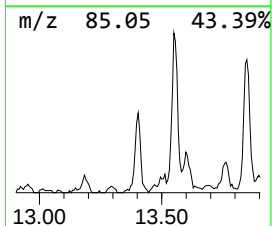
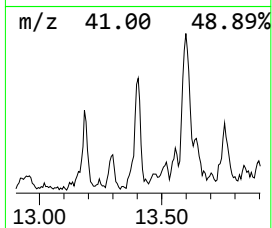
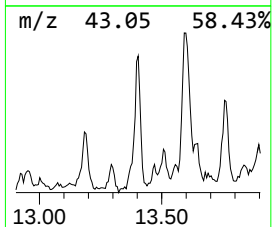
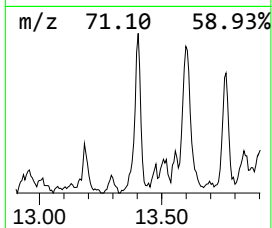
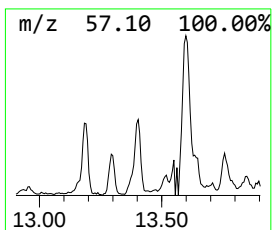
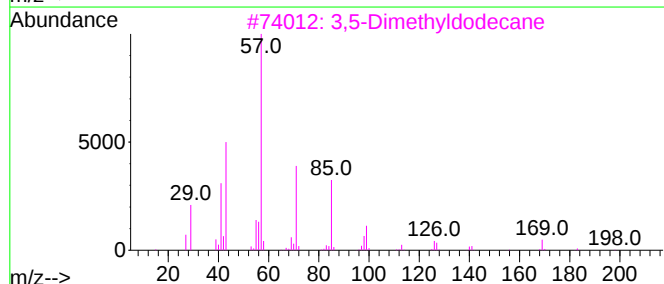
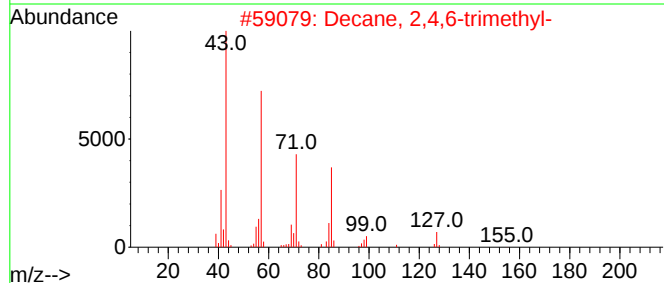
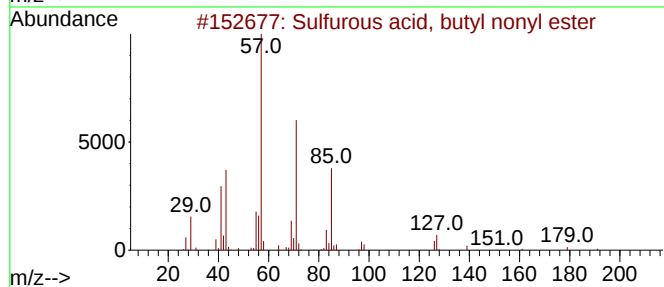
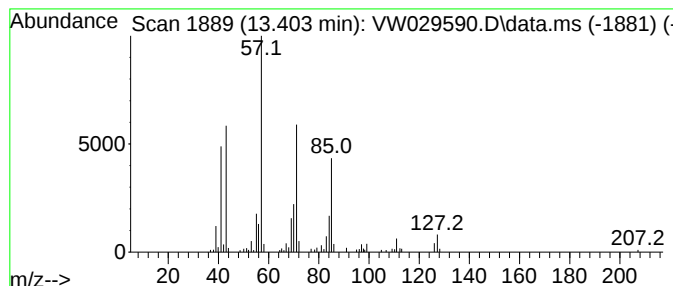
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM070824SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 Sulfurous acid, butyl nonyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.403	1.29 ug/L	53153	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	72
2			Decane, 2,4,6-trimethyl-	184	C13H28	062108-27-4	64
3			3,5-Dimethyldodecane	198	C14H30	107770-99-0	59
4			Pentan-2-yl 2-methylbutanoate	172	C10H20O2	1000372-71-7	59
5			1-Iodo-2-methylnonane	268	C10H21I	1000101-47-9	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfurous acid,...	13.403	1.3	ug/L	53153	3	13.556	1026530	25.0