

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW071124\
 Data File : VW029532.D
 Acq On : 11 Jul 2024 16:22
 Operator : SY/MD
 Sample : P3178-12
 Misc : 5.30g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 A4BT7

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: VW029532.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.210	51	53	54	rBV2	1001	698	0.05%	0.006%
2	2.363	72	78	95	rVB	81737	193159	12.97%	1.685%
3	2.625	119	121	125	rBV5	2085	3482	0.23%	0.030%
4	2.899	158	166	182	rBV	57546	168138	11.29%	1.467%
5	3.399	243	248	251	rVB5	1050	1840	0.12%	0.016%
6	3.472	258	260	262	rBV2	361	399	0.03%	0.003%
7	3.509	264	266	268	rVV3	445	479	0.03%	0.004%
8	3.576	276	277	280	rVB2	412	434	0.03%	0.004%
9	3.716	298	300	301	rBV2	627	485	0.03%	0.004%
10	4.021	339	350	364	rBV	148684	487569	32.75%	4.253%
11	4.265	388	390	392	rVB3	444	464	0.03%	0.004%
12	4.387	407	410	413	rBV3	414	658	0.04%	0.006%
13	4.618	445	448	451	rBV3	530	602	0.04%	0.005%
14	4.917	485	497	510	rVV	16775	64381	4.32%	0.562%
15	5.161	525	537	547	rBV5	2548	9514	0.64%	0.083%
16	5.362	569	570	574	rBV3	411	428	0.03%	0.004%
17	5.539	598	599	602	rVB2	456	429	0.03%	0.004%
18	5.618	607	612	613	rBV3	348	562	0.04%	0.005%
19	5.716	625	628	629	rBV3	485	414	0.03%	0.004%
20	5.734	629	631	634	rVV3	608	664	0.04%	0.006%
21	5.764	634	636	639	rVB4	753	636	0.04%	0.006%
22	5.941	654	665	678	rVV2	7348	23250	1.56%	0.203%
23	6.167	700	702	704	rBV2	633	671	0.05%	0.006%
24	6.362	732	734	738	rBV2	376	517	0.03%	0.005%
25	6.636	776	779	782	rVB3	635	645	0.04%	0.006%
26	6.917	816	825	826	rBV4	1568	2724	0.18%	0.024%
27	7.075	842	851	867	rBV	33349	106007	7.12%	0.925%
28	7.307	886	889	890	rVB2	481	404	0.03%	0.004%
29	7.410	904	906	909	rBV2	473	409	0.03%	0.004%
30	7.545	925	928	932	rVV4	542	880	0.06%	0.008%
31	7.648	934	945	958	rVV	239724	588790	39.55%	5.136%
32	7.758	961	963	970	rVV5	1351	2539	0.17%	0.022%
33	7.898	983	986	988	rBV3	484	518	0.03%	0.005%
34	7.935	988	992	993	rVB3	692	710	0.05%	0.006%
35	8.032	1004	1008	1009	rBV2	348	503	0.03%	0.004%
36	8.276	1036	1048	1066	rBV2	484359	1421385	95.47%	12.399%

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

37	8.398	1066	1068	1075	rVB6	1297	2249	0.15%	0.020%
38	8.526	1085	1089	1091	rBV2	811	920	0.06%	0.008%
39	8.605	1099	1102	1103	rBV	476	551	0.04%	0.005%
40	8.624	1103	1105	1107	rBV2	367	465	0.03%	0.004%
41	8.843	1131	1141	1157	rBV	635692	1258969	84.56%	10.982%
42	9.063	1170	1177	1178	rBV7	1770	3400	0.23%	0.030%
43	9.154	1190	1192	1196	rVB4	463	397	0.03%	0.003%
44	9.185	1196	1197	1200	rBV3	416	439	0.03%	0.004%
45	9.270	1202	1211	1221	rBV	328299	671599	45.11%	5.858%
46	9.666	1272	1276	1285	rVB4	697	1848	0.12%	0.016%
47	9.965	1322	1325	1327	rBV2	461	538	0.04%	0.005%
48	10.032	1327	1336	1345	rBV	169072	305912	20.55%	2.668%
49	10.130	1350	1352	1353	rBV	771	489	0.03%	0.004%
50	10.325	1375	1384	1392	rBV	662433	1188516	79.83%	10.367%
51	10.386	1392	1394	1398	rVB2	6037	8157	0.55%	0.071%
52	10.507	1411	1414	1416	rVB3	590	687	0.05%	0.006%
53	10.575	1416	1425	1435	rBV	101330	182744	12.27%	1.594%
54	10.703	1440	1446	1453	rVB3	3171	6589	0.44%	0.057%
55	10.837	1464	1468	1469	rBV4	840	1073	0.07%	0.009%
56	10.922	1475	1482	1493	rBV	128667	226194	15.19%	1.973%
57	11.081	1504	1508	1514	rVB6	789	1557	0.10%	0.014%
58	11.160	1519	1521	1522	rBV2	639	498	0.03%	0.004%
59	11.178	1522	1524	1527	rVB	1077	944	0.06%	0.008%
60	11.294	1541	1543	1546	rBV3	358	430	0.03%	0.004%
61	11.398	1558	1560	1566	rVV5	994	1256	0.08%	0.011%
62	11.629	1589	1598	1608	rBV	882453	1488829	100.00%	12.987%
63	11.837	1627	1632	1638	rVB3	3280	6060	0.41%	0.053%
64	12.160	1681	1685	1693	rVB4	2080	4141	0.28%	0.036%
65	12.221	1693	1695	1697	rBV3	503	492	0.03%	0.004%
66	12.349	1714	1716	1720	rVB4	865	877	0.06%	0.008%
67	12.471	1732	1736	1739	rVV5	1512	2110	0.14%	0.018%
68	12.519	1742	1744	1746	rVV3	622	473	0.03%	0.004%
69	12.592	1750	1756	1764	rVB5	11692	23678	1.59%	0.207%
70	12.690	1764	1772	1779	rBV	208884	349781	23.49%	3.051%
71	12.751	1779	1782	1794	rVB5	3566	8912	0.60%	0.078%
72	12.867	1798	1801	1803	rBV3	791	1098	0.07%	0.010%
73	12.952	1807	1815	1822	rBV8	3711	9879	0.66%	0.086%
74	13.007	1822	1824	1828	rBV5	818	1173	0.08%	0.010%
75	13.086	1830	1837	1838	rBV4	1523	2253	0.15%	0.020%
76	13.190	1846	1854	1859	rVB	26889	43824	2.94%	0.382%

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 Title : SFAM01.0

77	13.294	1865	1871	1880	rVB	12012	22786	1.53%	0.199%
78	13.403	1880	1889	1896	rBV	40469	78176	5.25%	0.682%
79	13.470	1896	1900	1902	rBV5	4188	5715	0.38%	0.050%
80	13.556	1902	1914	1919	rBV	872466	1442761	96.91%	12.585%
81	13.757	1941	1947	1955	rVB3	29958	57671	3.87%	0.503%
82	13.848	1955	1962	1968	rBV	546980	892873	59.97%	7.789%
83	14.062	1993	1997	2000	rBV2	11095	17465	1.17%	0.152%
84	14.171	2013	2015	2020	rBV5	974	1147	0.08%	0.010%
85	14.251	2026	2028	2032	rBV3	1384	1977	0.13%	0.017%
86	14.318	2036	2039	2045	rVB4	8011	11719	0.79%	0.102%
87	14.495	2063	2068	2079	rVB5	5235	13737	0.92%	0.120%
88	14.684	2097	2099	2102	rBV3	1803	1984	0.13%	0.017%
89	15.019	2150	2154	2158	rBV5	914	1489	0.10%	0.013%
90	15.092	2164	2166	2169	rVB4	1089	917	0.06%	0.008%
91	15.391	2211	2215	2222	rVB4	6017	10184	0.68%	0.089%
92	15.671	2258	2261	2266	rVB7	1314	2369	0.16%	0.021%
93	16.086	2328	2329	2333	rVB3	1082	860	0.06%	0.008%
94	16.202	2346	2348	2350	rBV3	697	606	0.04%	0.005%
95	16.311	2365	2366	2369	rBV3	722	778	0.05%	0.007%
96	16.342	2369	2371	2373	rVV	640	542	0.04%	0.005%
97	16.403	2378	2381	2382	rBV3	1000	992	0.07%	0.009%
98	16.549	2403	2405	2407	rBV3	723	663	0.04%	0.006%
99	16.604	2412	2414	2416	rBV2	859	704	0.05%	0.006%
100	16.695	2427	2429	2432	rBV4	495	418	0.03%	0.004%

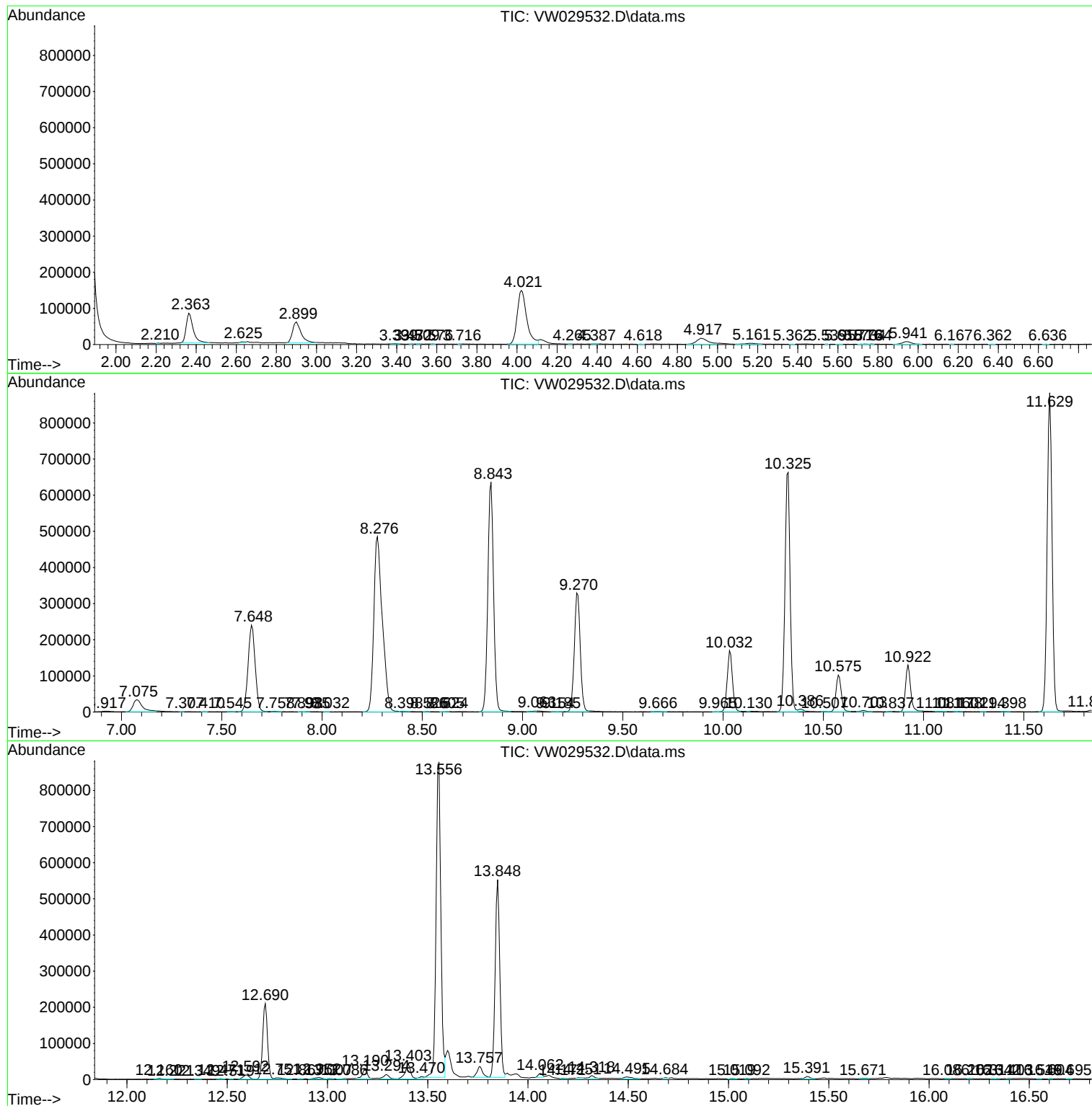
Sum of corrected areas: 11463921

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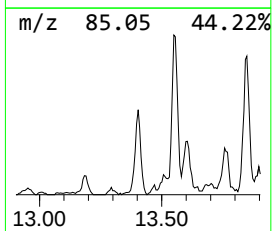
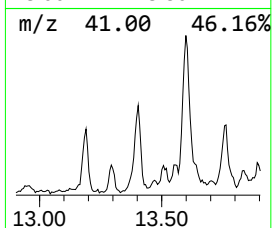
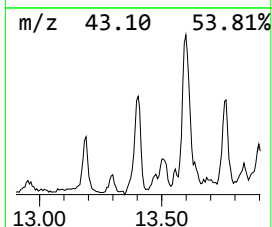
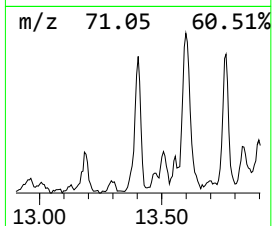
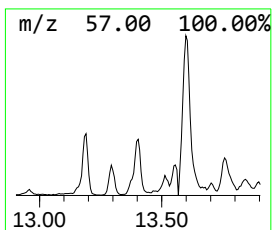
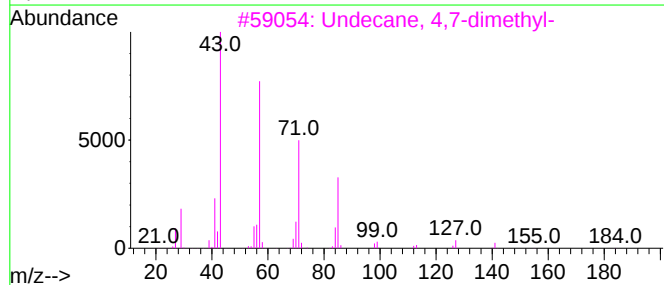
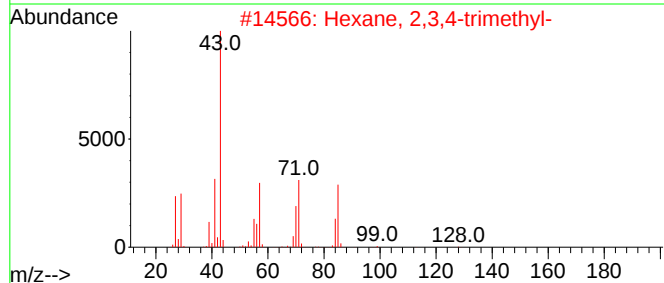
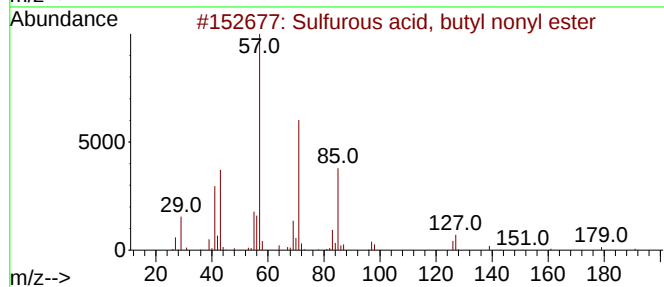
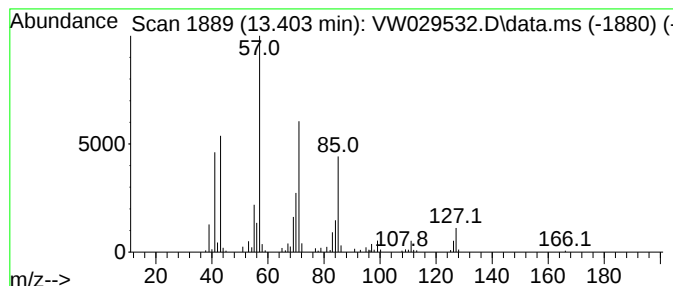
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM070824SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 Sulfurous acid, butyl nonyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.403	1.35 ug/L	78176	1,4-Dichlorobenzene-d4	13.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	72
2			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	53
3			Undecane, 4,7-dimethyl-	184	C13H28	017301-32-5	53
4			Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	50
5			Undecane, 2,4-dimethyl-	184	C13H28	017312-80-0	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfurous acid,...	13.403	1.4	ug/L	78176	3	13.550	1442760	25.0