

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW071624\
 Data File : VW029597.D
 Acq On : 16 Jul 2024 18:08
 Operator : SY/MD
 Sample : P3263-07
 Misc : 5.20g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 A4BB0

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: VW029597.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.223	51	55	56	rBV2	1823	1867	0.14%	0.021%
2	2.363	72	78	95	rBV	44095	128628	9.85%	1.424%
3	2.899	159	166	180	rBV	37721	117972	9.03%	1.306%
4	3.338	236	238	242	rBV3	568	899	0.07%	0.010%
5	3.411	248	250	254	rVB3	664	802	0.06%	0.009%
6	3.533	267	270	272	rBV3	622	822	0.06%	0.009%
7	3.637	285	287	291	rVB4	586	736	0.06%	0.008%
8	3.704	294	298	299	rBV4	697	853	0.07%	0.009%
9	4.021	339	350	374	rVV	97797	352836	27.02%	3.907%
10	4.454	419	421	425	rVB4	630	825	0.06%	0.009%
11	4.606	442	446	447	rBV4	722	835	0.06%	0.009%
12	4.734	463	467	471	rVB4	455	665	0.05%	0.007%
13	4.795	475	477	481	rBV4	439	678	0.05%	0.008%
14	4.923	486	498	518	rBV2	25729	110221	8.44%	1.221%
15	5.387	570	574	576	rVB3	530	649	0.05%	0.007%
16	5.441	580	583	589	rVB6	844	1440	0.11%	0.016%
17	5.643	612	616	618	rBV4	450	734	0.06%	0.008%
18	5.856	648	651	652	rBV2	579	680	0.05%	0.008%
19	5.948	654	666	676	rVV3	7579	24485	1.87%	0.271%
20	6.106	689	692	698	rBV4	612	1130	0.09%	0.013%
21	6.356	730	733	737	rBV3	411	675	0.05%	0.007%
22	6.460	745	750	752	rVB3	360	705	0.05%	0.008%
23	6.533	760	762	765	rVB3	846	679	0.05%	0.008%
24	6.582	765	770	772	rBV4	747	1302	0.10%	0.014%
25	6.899	820	822	825	rVB3	537	647	0.05%	0.007%
26	7.075	843	851	874	rBV2	23756	95256	7.29%	1.055%
27	7.386	899	902	903	rVB3	774	765	0.06%	0.008%
28	7.563	929	931	934	rVB3	1087	929	0.07%	0.010%
29	7.648	934	945	959	rBV	192571	469657	35.96%	5.201%
30	7.752	959	962	963	rBV3	973	1046	0.08%	0.012%
31	7.947	992	994	998	rVV4	595	894	0.07%	0.010%
32	8.069	1010	1014	1015	rBV3	585	656	0.05%	0.007%
33	8.276	1036	1048	1067	rBV2	373440	1099179	84.16%	12.172%
34	8.404	1067	1069	1072	rVB3	869	690	0.05%	0.008%
35	8.697	1110	1117	1122	rBV7	1898	3999	0.31%	0.044%
36	8.843	1132	1141	1152	rBV	563931	1135406	86.94%	12.573%

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 Title : SFAM01.0

37	9.026	1169	1171	1173	rBV3	795	794	0.06%	0.009%
38	9.087	1173	1181	1186	rVB3	2573	6555	0.50%	0.073%
39	9.270	1201	1211	1222	rBV	260943	543465	41.61%	6.018%
40	9.429	1235	1237	1240	rVB3	829	879	0.07%	0.010%
41	9.471	1240	1244	1246	rBV4	789	779	0.06%	0.009%
42	9.794	1293	1297	1300	rVB2	475	641	0.05%	0.007%
43	9.868	1306	1309	1310	rBV3	726	805	0.06%	0.009%
44	10.032	1326	1336	1349	rBV	116271	215126	16.47%	2.382%
45	10.239	1368	1370	1374	rBV4	580	676	0.05%	0.007%
46	10.319	1375	1383	1392	rBV	481577	836041	64.02%	9.258%
47	10.502	1411	1413	1417	rBV4	1034	1323	0.10%	0.015%
48	10.575	1418	1425	1436	rBV	75353	130978	10.03%	1.450%
49	10.703	1440	1446	1451	rVB	4485	9093	0.70%	0.101%
50	10.764	1453	1456	1458	rBV3	876	1371	0.10%	0.015%
51	10.861	1464	1472	1476	rBV4	10943	22715	1.74%	0.252%
52	10.922	1476	1482	1495	rVV	95365	181594	13.90%	2.011%
53	11.178	1520	1524	1529	rVB7	1764	3211	0.25%	0.036%
54	11.276	1537	1540	1543	rBV5	625	1137	0.09%	0.013%
55	11.331	1546	1549	1554	rVB3	1465	2244	0.17%	0.025%
56	11.398	1556	1560	1571	rVB8	2499	4992	0.38%	0.055%
57	11.532	1579	1582	1586	rBV5	758	1305	0.10%	0.014%
58	11.629	1589	1598	1606	rBV	773009	1306001	100.00%	14.462%
59	11.831	1629	1631	1633	rBV3	887	1097	0.08%	0.012%
60	11.873	1634	1638	1644	rVB4	4015	7375	0.56%	0.082%
61	12.068	1667	1670	1672	rBV3	1022	1269	0.10%	0.014%
62	12.184	1682	1689	1691	rBV5	1342	2704	0.21%	0.030%
63	12.361	1715	1718	1720	rVV4	1050	1114	0.09%	0.012%
64	12.428	1726	1729	1730	rVB3	945	823	0.06%	0.009%
65	12.465	1730	1735	1740	rBV6	1933	3882	0.30%	0.043%
66	12.593	1747	1756	1763	rBV3	10973	24415	1.87%	0.270%
67	12.690	1764	1772	1779	rVV	179291	294875	22.58%	3.265%
68	12.745	1779	1781	1792	rVB7	3944	10630	0.81%	0.118%
69	12.830	1792	1795	1796	rBV3	1159	1065	0.08%	0.012%
70	12.867	1799	1801	1802	rVV2	941	746	0.06%	0.008%
71	12.879	1802	1803	1806	rVV2	1052	1194	0.09%	0.013%
72	12.958	1807	1816	1821	rVV8	4119	12208	0.93%	0.135%
73	13.001	1821	1823	1829	rVB4	1429	2330	0.18%	0.026%
74	13.086	1834	1837	1838	rBV2	779	885	0.07%	0.010%
75	13.123	1840	1843	1845	rBV4	1212	1669	0.13%	0.018%
76	13.184	1845	1853	1864	rVB	20696	41554	3.18%	0.460%

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 Title : SFAM01.0

77	13.294	1864	1871	1878	rBV2	10906	18099	1.39%	0.200%
78	13.403	1880	1889	1895	rBV	34533	63147	4.84%	0.699%
79	13.464	1895	1899	1902	rBV4	3801	5982	0.46%	0.066%
80	13.556	1907	1914	1919	rBV	661576	1050807	80.46%	11.636%
81	13.757	1941	1947	1954	rVB2	20231	37384	2.86%	0.414%
82	13.849	1955	1962	1968	rBV	345332	575383	44.06%	6.372%
83	14.519	2064	2072	2082	rBV3	5934	12806	0.98%	0.142%
84	14.629	2087	2090	2093	rVV4	748	1277	0.10%	0.014%
85	14.696	2096	2101	2102	rBV3	984	1667	0.13%	0.018%
86	14.720	2102	2105	2109	rVB5	1438	1965	0.15%	0.022%
87	14.836	2122	2124	2126	rBV3	665	665	0.05%	0.007%
88	15.202	2177	2184	2187	rBV6	2794	5904	0.45%	0.065%
89	15.245	2187	2191	2195	rVB7	2051	4166	0.32%	0.046%
90	15.397	2215	2216	2220	rVB4	1093	896	0.07%	0.010%
91	15.592	2247	2248	2251	rBV3	944	1078	0.08%	0.012%
92	15.879	2293	2295	2297	rVB3	736	693	0.05%	0.008%
93	15.934	2301	2304	2305	rBV2	663	750	0.06%	0.008%
94	15.988	2312	2313	2317	rVB4	944	861	0.07%	0.010%
95	16.031	2317	2320	2324	rVB5	766	995	0.08%	0.011%
96	16.104	2330	2332	2335	rVB3	619	690	0.05%	0.008%
97	16.208	2346	2349	2352	rBV3	826	1028	0.08%	0.011%
98	16.305	2363	2365	2368	rVB4	582	679	0.05%	0.008%
99	16.342	2368	2371	2373	rBV3	613	835	0.06%	0.009%
100	16.653	2419	2422	2424	rVV4	657	778	0.06%	0.009%

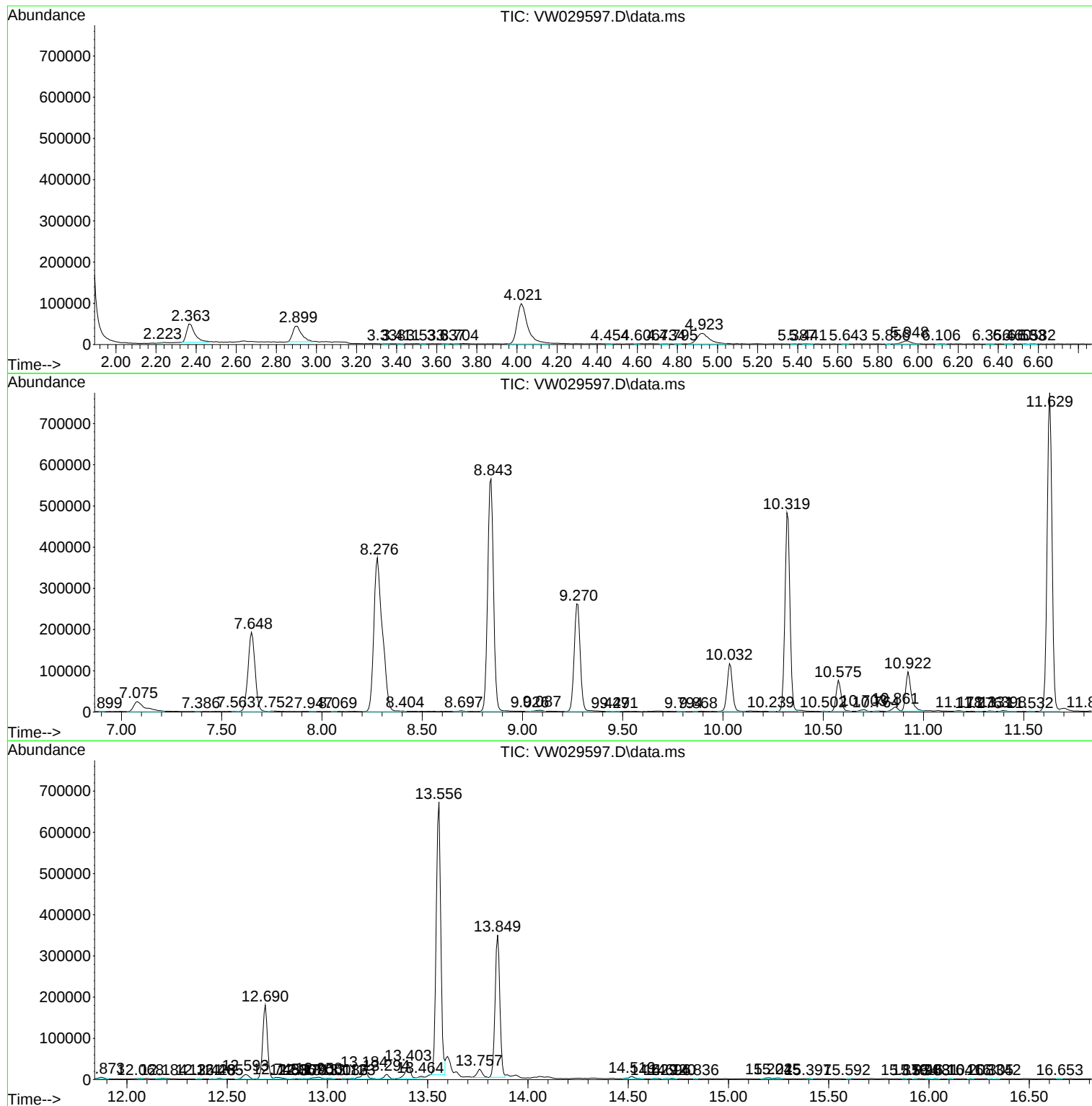
Sum of corrected areas: 9030337

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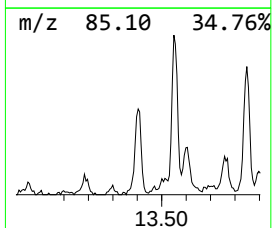
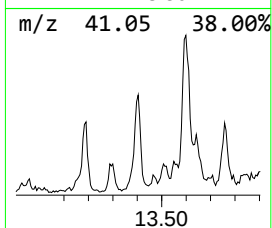
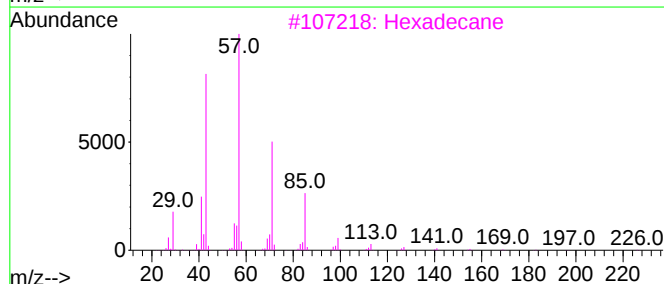
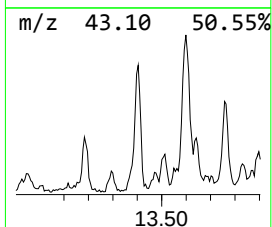
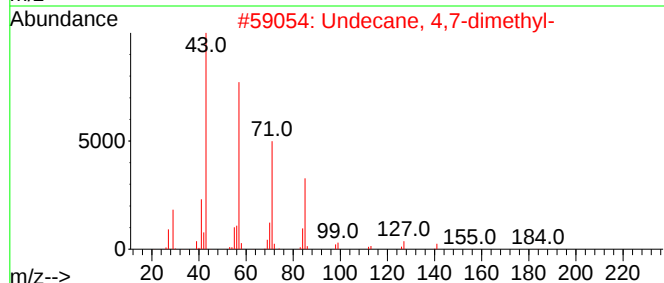
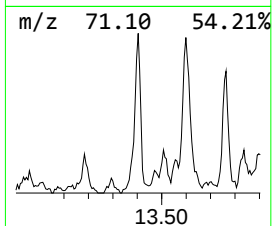
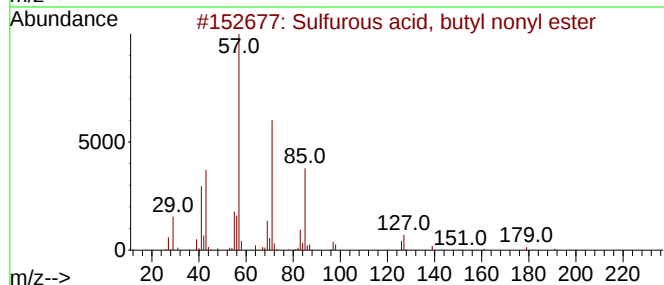
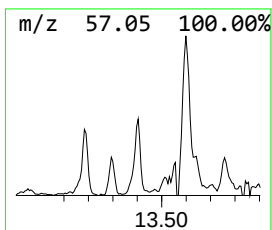
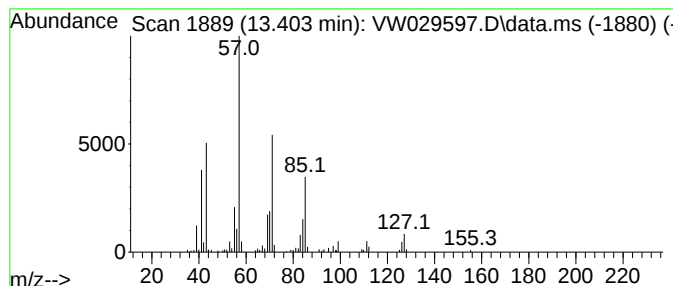
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM070824SMA.M
Quant Title : SFAM01.0

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	1.50 ug/L	63147	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			Undecane, 4,7-dimethyl-	184	C13H28	017301-32-5	59
3			Hexadecane	226	C16H34	000544-76-3	59
4			Oxalic acid, isohexyl neopentyl ...	244	C13H24O4	1000309-73-0	50
5			Octane, 6-ethyl-2-methyl-	156	C11H24	062016-19-7	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfurous acid,...	13.403	1.5	ug/L	63147	3	13.556	1050810	25.0