

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW101222\
 Data File : VW024875.D
 Acq On : 12 Oct 2022 15:58
 Operator : SY/VA
 Sample : N5070-01
 Misc : 5.37g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 C0BK4

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\SFAMWLM101222SMA.M
 Title : SFAM01.0

Signal : TIC: VW024875.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.355	68	74	85	rVB	122948	198851	10.92%	1.636%
2	2.885	155	161	169	rBV	67601	137603	7.56%	1.132%
3	3.336	234	235	237	rBV	618	464	0.03%	0.004%
4	3.513	261	264	265	rBV2	493	529	0.03%	0.004%
5	3.586	274	276	278	rBV2	538	417	0.02%	0.003%
6	3.678	289	291	295	rVB2	510	657	0.04%	0.005%
7	3.769	304	306	309	rVB2	334	264	0.01%	0.002%
8	3.842	315	318	319	rVB2	398	332	0.02%	0.003%
9	3.903	326	328	329	rVB	538	284	0.02%	0.002%
10	4.019	335	347	361	rBV2	182856	552949	30.37%	4.548%
11	4.361	400	403	404	rBV2	267	309	0.02%	0.003%
12	4.373	404	405	408	rVV3	546	583	0.03%	0.005%
13	4.422	411	413	414	rVB	600	321	0.02%	0.003%
14	4.623	438	446	450	rBV2	3008	7725	0.42%	0.064%
15	4.921	482	495	509	rBV2	38923	129755	7.13%	1.067%
16	5.092	521	523	524	rBV2	478	413	0.02%	0.003%
17	5.275	551	553	554	rVV2	311	259	0.01%	0.002%
18	5.318	558	560	562	rVV	283	253	0.01%	0.002%
19	5.354	562	566	568	rVB2	231	284	0.02%	0.002%
20	5.379	568	570	571	rBV2	498	342	0.02%	0.003%
21	5.446	579	581	584	rVV2	586	558	0.03%	0.005%
22	5.537	594	596	598	rVB2	291	270	0.01%	0.002%
23	5.714	624	625	630	rBV2	273	392	0.02%	0.003%
24	5.848	644	647	649	rBV2	289	316	0.02%	0.003%
25	5.866	649	650	652	rVB2	480	288	0.02%	0.002%
26	5.946	652	663	672	rBV2	9119	28033	1.54%	0.231%
27	6.074	682	684	687	rVB	431	453	0.02%	0.004%
28	6.104	687	689	691	rBV2	351	341	0.02%	0.003%
29	6.299	720	721	724	rBV2	349	357	0.02%	0.003%
30	6.342	724	728	729	rVB2	316	269	0.01%	0.002%
31	6.439	742	744	746	rBV	464	521	0.03%	0.004%
32	6.543	760	761	767	rBV	324	406	0.02%	0.003%
33	6.604	769	771	774	rBV2	347	336	0.02%	0.003%
34	6.811	803	805	807	rBV	376	257	0.01%	0.002%
35	6.909	817	821	822	rBV2	243	320	0.02%	0.003%
36	7.080	840	849	874	rBV	47469	168337	9.25%	1.385%

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 Title : SFAM01.0

37	7.378	896	898	903	rBV3	331	568	0.03%	0.005%
38	7.439	907	908	911	rBV	407	456	0.03%	0.004%
39	7.647	931	942	955	rBV	332437	826171	45.38%	6.796%
40	7.811	968	969	972	rBV2	379	317	0.02%	0.003%
41	7.842	972	974	976	rVB	404	282	0.02%	0.002%
42	7.866	976	978	980	rBV2	403	396	0.02%	0.003%
43	7.957	986	993	996	rBV4	435	1063	0.06%	0.009%
44	8.079	1011	1013	1016	rVB	374	341	0.02%	0.003%
45	8.274	1035	1045	1060	rBV2	607734	1820554	100.00%	14.975%
46	8.689	1112	1113	1115	rBV2	371	332	0.02%	0.003%
47	8.841	1128	1138	1157	rVV	678466	1310824	72.00%	10.783%
48	8.988	1160	1162	1165	rVB2	318	316	0.02%	0.003%
49	9.079	1170	1177	1184	rVB4	2015	4610	0.25%	0.038%
50	9.177	1191	1193	1195	rVB	415	267	0.01%	0.002%
51	9.274	1197	1209	1218	rBV	466166	923098	50.70%	7.593%
52	9.421	1232	1233	1236	rBV	385	435	0.02%	0.004%
53	9.658	1269	1272	1284	rVB5	1679	4486	0.25%	0.037%
54	9.786	1290	1293	1297	rBV	401	549	0.03%	0.005%
55	9.896	1308	1311	1314	rBV3	249	397	0.02%	0.003%
56	10.036	1325	1334	1343	rBV	143976	266796	14.65%	2.195%
57	10.213	1361	1363	1365	rBV2	373	294	0.02%	0.002%
58	10.323	1371	1381	1388	rBV	761596	1350202	74.16%	11.106%
59	10.579	1416	1423	1433	rBV	87182	152878	8.40%	1.258%
60	10.701	1439	1443	1447	rVB4	2297	3434	0.19%	0.028%
61	10.859	1466	1469	1473	rBV3	978	1497	0.08%	0.012%
62	10.926	1473	1480	1494	rBV	152313	277616	15.25%	2.284%
63	11.231	1527	1530	1534	rBV2	309	440	0.02%	0.004%
64	11.298	1536	1541	1542	rVB3	396	589	0.03%	0.005%
65	11.311	1542	1543	1545	rBV	283	257	0.01%	0.002%
66	11.396	1554	1557	1558	rBV2	378	260	0.01%	0.002%
67	11.628	1587	1595	1606	rBV	797949	1370238	75.26%	11.271%
68	11.798	1622	1623	1624	rBV	685	290	0.02%	0.002%
69	11.841	1624	1630	1635	rVV6	3751	7046	0.39%	0.058%
70	11.993	1652	1655	1660	rBV3	350	608	0.03%	0.005%
71	12.085	1668	1670	1673	rBV	703	783	0.04%	0.006%
72	12.170	1678	1684	1693	rVV6	3394	7200	0.40%	0.059%
73	12.310	1703	1707	1709	rBV2	410	531	0.03%	0.004%
74	12.365	1712	1716	1718	rBV3	523	653	0.04%	0.005%
75	12.414	1722	1724	1728	rVB	340	307	0.02%	0.003%
76	12.457	1728	1731	1733	rBV	1127	1320	0.07%	0.011%

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 Title : SFAM01.0

77	12.603	1748	1755	1762	rVV4	9374	17388	0.96%	0.143%
78	12.688	1762	1769	1777	rBV	330245	545229	29.95%	4.485%
79	12.798	1785	1787	1788	rBV	550	345	0.02%	0.003%
80	12.871	1793	1799	1801	rBV2	820	1365	0.07%	0.011%
81	12.932	1807	1809	1817	rVB3	3044	4976	0.27%	0.041%
82	13.091	1832	1835	1836	rBV	624	575	0.03%	0.005%
83	13.109	1836	1838	1840	rVB	708	459	0.03%	0.004%
84	13.127	1840	1841	1844	rBV2	286	416	0.02%	0.003%
85	13.243	1854	1860	1878	rBV3	29609	60186	3.31%	0.495%
86	13.499	1898	1902	1904	rBV3	1649	2001	0.11%	0.016%
87	13.554	1904	1911	1919	rVV	692434	1078649	59.25%	8.873%
88	13.853	1952	1960	1967	rBV	509810	848993	46.63%	6.984%
89	14.066	1990	1995	2000	rVB2	6382	9637	0.53%	0.079%
90	14.365	2042	2044	2045	rBV2	446	344	0.02%	0.003%
91	14.420	2051	2053	2055	rBV3	448	367	0.02%	0.003%
92	14.627	2083	2087	2090	rVB5	1107	1766	0.10%	0.015%
93	14.682	2094	2096	2099	rVV3	470	338	0.02%	0.003%
94	14.718	2099	2102	2108	rVV5	1198	1743	0.10%	0.014%
95	14.786	2111	2113	2114	rBV2	386	365	0.02%	0.003%
96	14.907	2131	2133	2134	rBV2	752	482	0.03%	0.004%
97	15.121	2166	2168	2174	rBV5	1096	1571	0.09%	0.013%
98	15.481	2222	2227	2231	rBV3	3060	5110	0.28%	0.042%
99	15.663	2255	2257	2258	rBV	574	359	0.02%	0.003%
100	15.791	2274	2278	2279	rBV3	923	1478	0.08%	0.012%

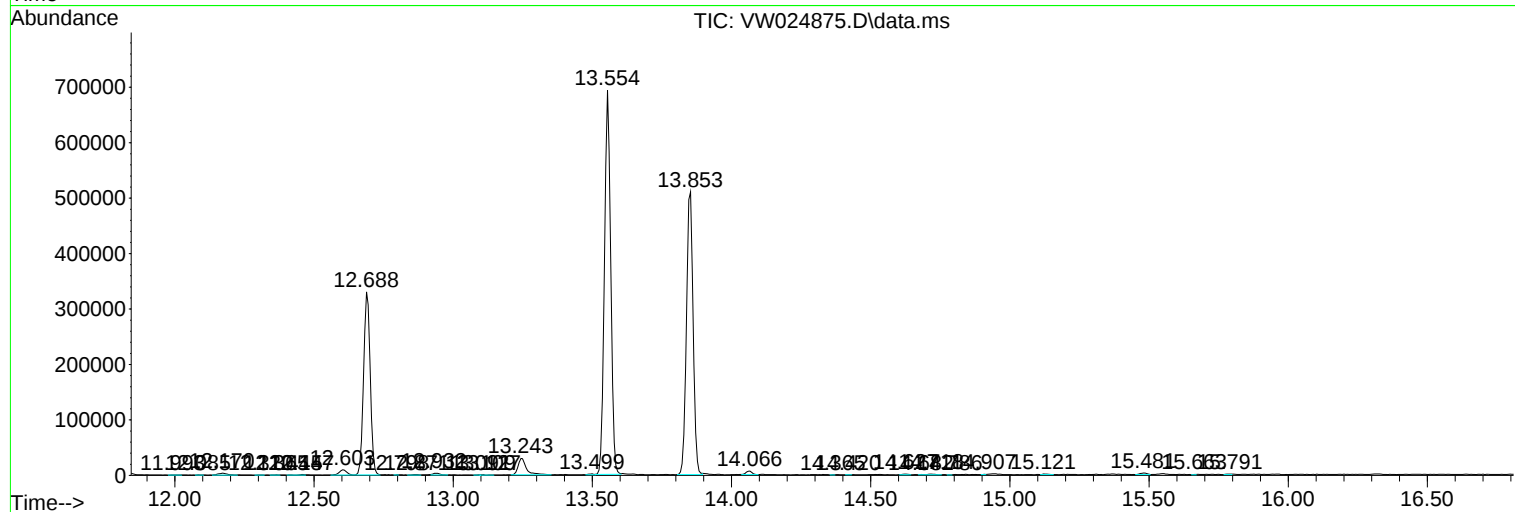
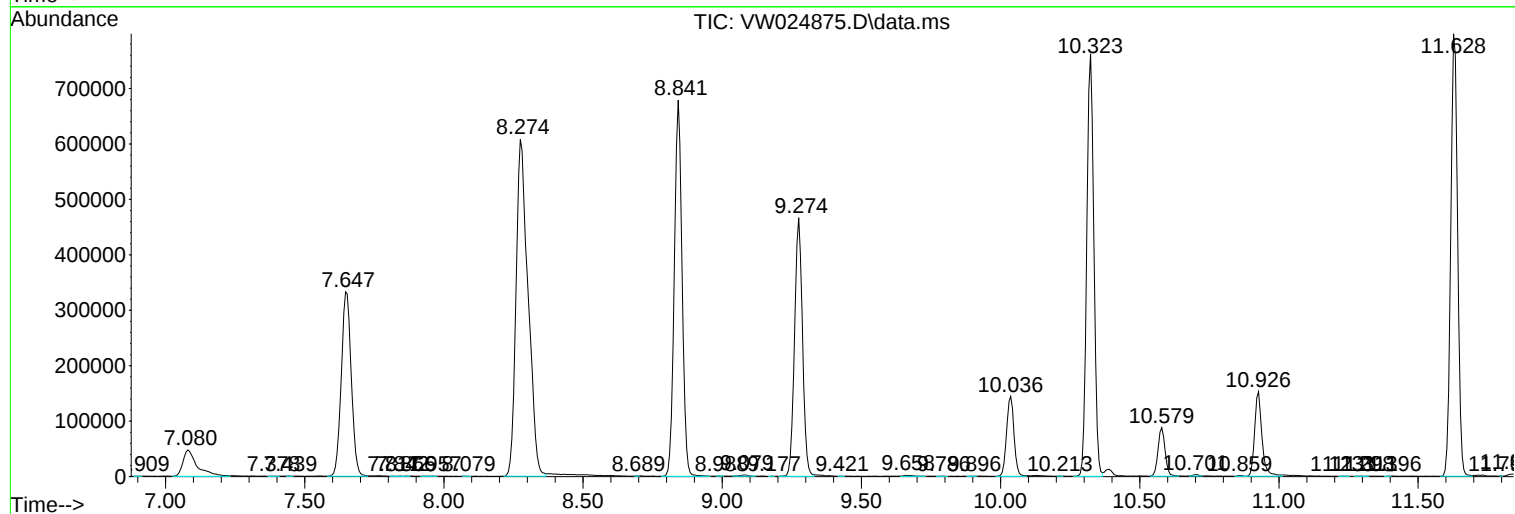
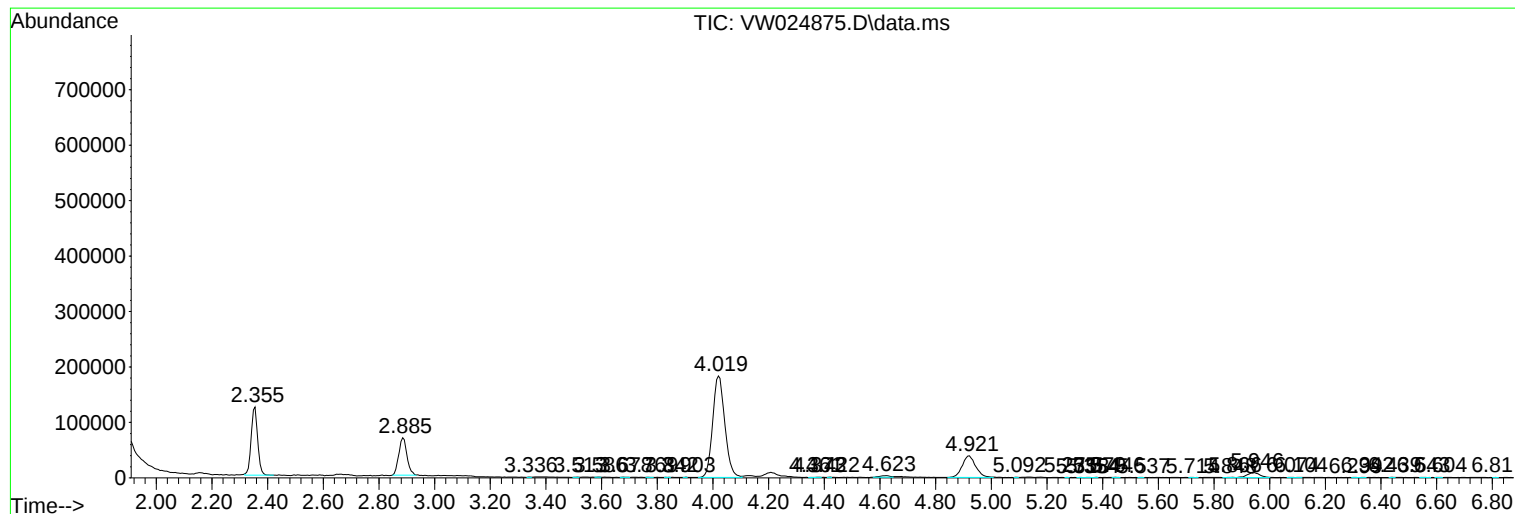
Sum of corrected areas: 12156891

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM101222SMA.M
Quant Title : SFAM01.0

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



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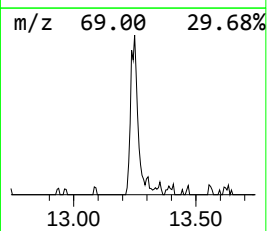
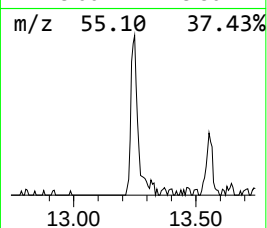
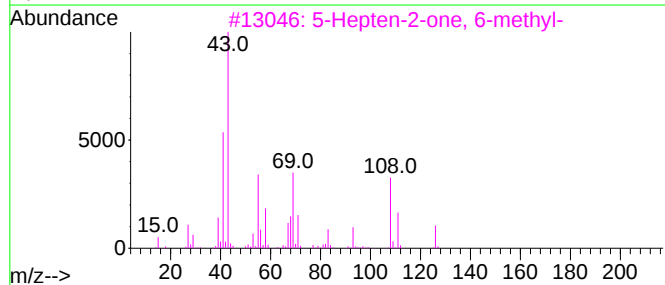
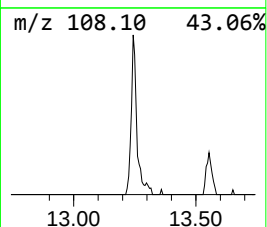
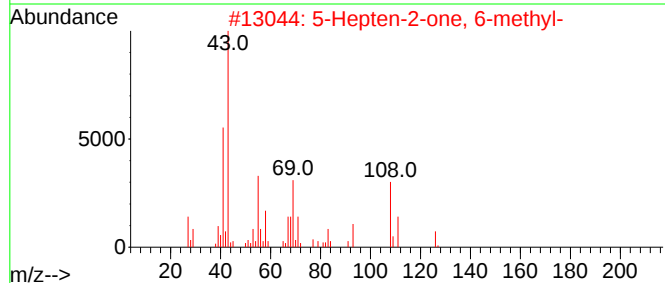
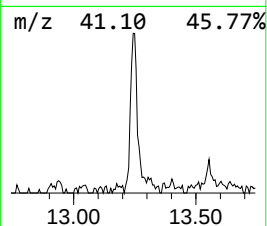
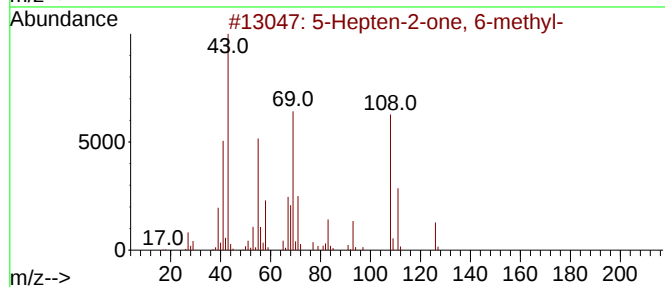
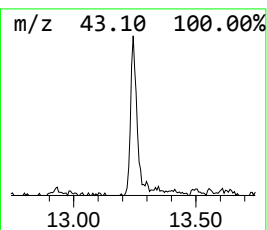
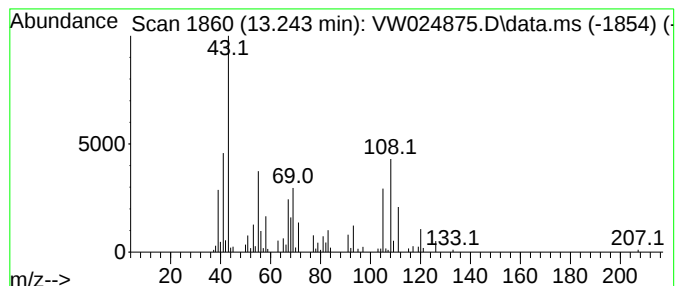
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM101222SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 5-Hepten-2-one, 6-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.243	1.39 ug/L	60186	1,4-Dichlorobenzene-d4	13.554

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Hepten-2-one, 6-methyl-	126	C8H14O	000110-93-0	53
2		5-Hepten-2-one, 6-methyl-	126	C8H14O	000110-93-0	43
3		5-Hepten-2-one, 6-methyl-	126	C8H14O	000110-93-0	38
4		5-Hepten-2-one, 6-methyl-	126	C8H14O	000110-93-0	38
5		5-Hepten-2-one, 6-methyl-	126	C8H14O	000110-93-0	37



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
5-Hepten-2-one,...	13.243	1.4	ug/L	60186	3	13.554	1078650	25.0