

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW061824\
 Data File : VW029188.D
 Acq On : 18 Jun 2024 19:13
 Operator : SY/MD
 Sample : P2934-01
 Misc : 5.03g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 A4B58

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\SFAMWLM061824SMA.M
 Title : SFAM01.0

Signal : TIC: VW029188.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.180	46	48	49	rBV2	1058	794	0.07%	0.012%
2	2.363	72	78	93	rBV	47180	127690	12.02%	1.884%
3	2.893	159	165	181	rVB	47502	133708	12.58%	1.973%
4	3.283	228	229	233	rVB4	917	1032	0.10%	0.015%
5	3.375	242	244	246	rBV3	985	1239	0.12%	0.018%
6	3.399	246	248	255	rVB7	2244	3050	0.29%	0.045%
7	3.472	257	260	261	rBV3	844	809	0.08%	0.012%
8	3.680	289	294	295	rBV5	871	1405	0.13%	0.021%
9	4.021	337	350	375	rBV	90257	334411	31.47%	4.935%
10	4.606	438	446	455	rBV	4028	12789	1.20%	0.189%
11	4.783	473	475	478	rBV3	822	988	0.09%	0.015%
12	4.929	485	499	514	rBV	21467	95036	8.94%	1.402%
13	5.137	528	533	535	rBV6	816	1411	0.13%	0.021%
14	5.386	572	574	577	rBV3	910	1012	0.10%	0.015%
15	5.612	609	611	614	rVB4	988	819	0.08%	0.012%
16	5.777	636	638	640	rBV3	1117	811	0.08%	0.012%
17	5.832	645	647	650	rVB3	832	786	0.07%	0.012%
18	5.941	655	665	673	rBV3	11227	35664	3.36%	0.526%
19	6.130	694	696	699	rVV4	729	955	0.09%	0.014%
20	6.191	703	706	709	rVV4	666	849	0.08%	0.013%
21	6.301	720	724	726	rBV5	1190	1553	0.15%	0.023%
22	6.319	726	727	731	rVV3	991	1019	0.10%	0.015%
23	6.368	731	735	736	rVV4	833	987	0.09%	0.015%
24	6.411	739	742	745	rVV5	773	1182	0.11%	0.017%
25	6.520	758	760	764	rVB3	590	873	0.08%	0.013%
26	6.636	776	779	782	rVB3	868	1109	0.10%	0.016%
27	6.661	782	783	786	rBV3	822	1058	0.10%	0.016%
28	6.911	822	824	826	rBV3	902	1102	0.10%	0.016%
29	6.947	828	830	835	rVB5	760	831	0.08%	0.012%
30	7.075	843	851	873	rBV	35252	124239	11.69%	1.833%
31	7.270	880	883	887	rVB6	856	1173	0.11%	0.017%
32	7.569	930	932	934	rBV3	769	858	0.08%	0.013%
33	7.648	934	945	956	rBV	195324	476005	44.79%	7.024%
34	7.825	973	974	978	rVB4	975	942	0.09%	0.014%
35	7.868	978	981	982	rBV2	777	762	0.07%	0.011%
36	8.026	1002	1007	1010	rVV6	767	1371	0.13%	0.020%

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 Title : SFAM01.0

37	8.276	1038	1048	1064	rBV2	340134	1062730	100.00%	15.682%
38	8.563	1091	1095	1096	rBV4	719	1044	0.10%	0.015%
39	8.843	1132	1141	1153	rVV	369977	744907	70.09%	10.992%
40	9.020	1169	1170	1173	rBV3	767	909	0.09%	0.013%
41	9.111	1184	1185	1189	rVB4	1051	937	0.09%	0.014%
42	9.270	1203	1211	1222	rBV	261645	537314	50.56%	7.929%
43	9.398	1230	1232	1236	rVB3	1100	933	0.09%	0.014%
44	9.465	1240	1243	1247	rVB5	817	1223	0.12%	0.018%
45	9.514	1247	1251	1254	rBV5	602	854	0.08%	0.013%
46	9.593	1261	1264	1266	rVB3	872	792	0.07%	0.012%
47	9.642	1270	1272	1273	rBV2	748	772	0.07%	0.011%
48	9.666	1273	1276	1277	rVV3	1030	1269	0.12%	0.019%
49	9.685	1277	1279	1283	rVB4	1130	1047	0.10%	0.015%
50	10.032	1326	1336	1345	rBV	73368	139213	13.10%	2.054%
51	10.123	1348	1351	1352	rBV2	1188	1049	0.10%	0.015%
52	10.325	1376	1384	1398	rVV	394122	703068	66.16%	10.375%
53	10.575	1419	1425	1433	rBV	51475	91571	8.62%	1.351%
54	10.703	1441	1446	1451	rVB2	6291	11418	1.07%	0.168%
55	10.843	1465	1469	1471	rBV4	835	1053	0.10%	0.016%
56	10.922	1475	1482	1494	rBV	85025	159657	15.02%	2.356%
57	11.135	1515	1517	1520	rBV4	987	994	0.09%	0.015%
58	11.190	1523	1526	1531	rVV6	1364	2844	0.27%	0.042%
59	11.629	1590	1598	1606	rBV	428440	706912	66.52%	10.432%
60	11.837	1627	1632	1639	rBV9	1938	4573	0.43%	0.067%
61	12.178	1684	1688	1694	rVB7	1276	3071	0.29%	0.045%
62	12.330	1712	1713	1716	rBV3	817	926	0.09%	0.014%
63	12.373	1718	1720	1723	rVB4	905	1090	0.10%	0.016%
64	12.465	1731	1735	1745	rVB9	3739	6427	0.60%	0.095%
65	12.544	1745	1748	1749	rVB3	918	859	0.08%	0.013%
66	12.599	1749	1757	1765	rBV3	19713	37879	3.56%	0.559%
67	12.690	1765	1772	1781	rBV	181300	297475	27.99%	4.390%
68	12.879	1796	1803	1805	rVV6	1216	2361	0.22%	0.035%
69	12.946	1809	1814	1820	rVV8	1499	4573	0.43%	0.067%
70	13.080	1832	1836	1837	rBV4	953	785	0.07%	0.012%
71	13.190	1846	1854	1857	rVV3	3889	6388	0.60%	0.094%
72	13.294	1868	1871	1875	rVB4	2289	3305	0.31%	0.049%
73	13.403	1882	1889	1894	rBV3	5794			

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 Title : SFAM01.0

77	13.763	1943	1948	1955	rVB6	4471	8296	0.78%	0.122%
78	13.848	1955	1962	1969	rBV	194402	325502	30.63%	4.803%
79	14.062	1990	1997	2002	rVV	9010	15597	1.47%	0.230%
80	14.318	2036	2039	2049	rVB8	3784	7853	0.74%	0.116%
81	14.421	2054	2056	2061	rVV6	705	1080	0.10%	0.016%
82	14.464	2061	2063	2065	rVV3	901	930	0.09%	0.014%
83	14.519	2067	2072	2081	rVV4	5498	10603	1.00%	0.156%
84	14.690	2096	2100	2101	rBV4	1336	1663	0.16%	0.025%
85	14.830	2121	2123	2125	rBV3	886	885	0.08%	0.013%
86	15.062	2156	2161	2167	rBV7	3691	7266	0.68%	0.107%
87	15.129	2169	2172	2175	rBV5	922	1205	0.11%	0.018%
88	15.196	2180	2183	2187	rVV3	2322	3942	0.37%	0.058%
89	15.238	2187	2190	2193	rVV4	1905	2922	0.27%	0.043%
90	15.342	2204	2207	2209	rBV3	643	820	0.08%	0.012%
91	15.476	2225	2229	2233	rVV5	1693	2831	0.27%	0.042%
92	15.537	2237	2239	2245	rBV6	652	1384	0.13%	0.020%
93	15.580	2245	2246	2251	rVB5	636	877	0.08%	0.013%
94	15.787	2278	2280	2284	rVB5	814	1149	0.11%	0.017%
95	15.958	2302	2308	2309	rBV5	1278	2358	0.22%	0.035%
96	16.086	2320	2329	2336	rBV4	9963	21609	2.03%	0.319%
97	16.317	2363	2367	2370	rVB6	666	845	0.08%	0.012%
98	16.409	2378	2382	2385	rBV4	760	1177	0.11%	0.017%
99	16.445	2385	2388	2390	rBV4	564	808	0.08%	0.012%
100	16.714	2429	2432	2435	rBV4	1075	1498	0.14%	0.022%

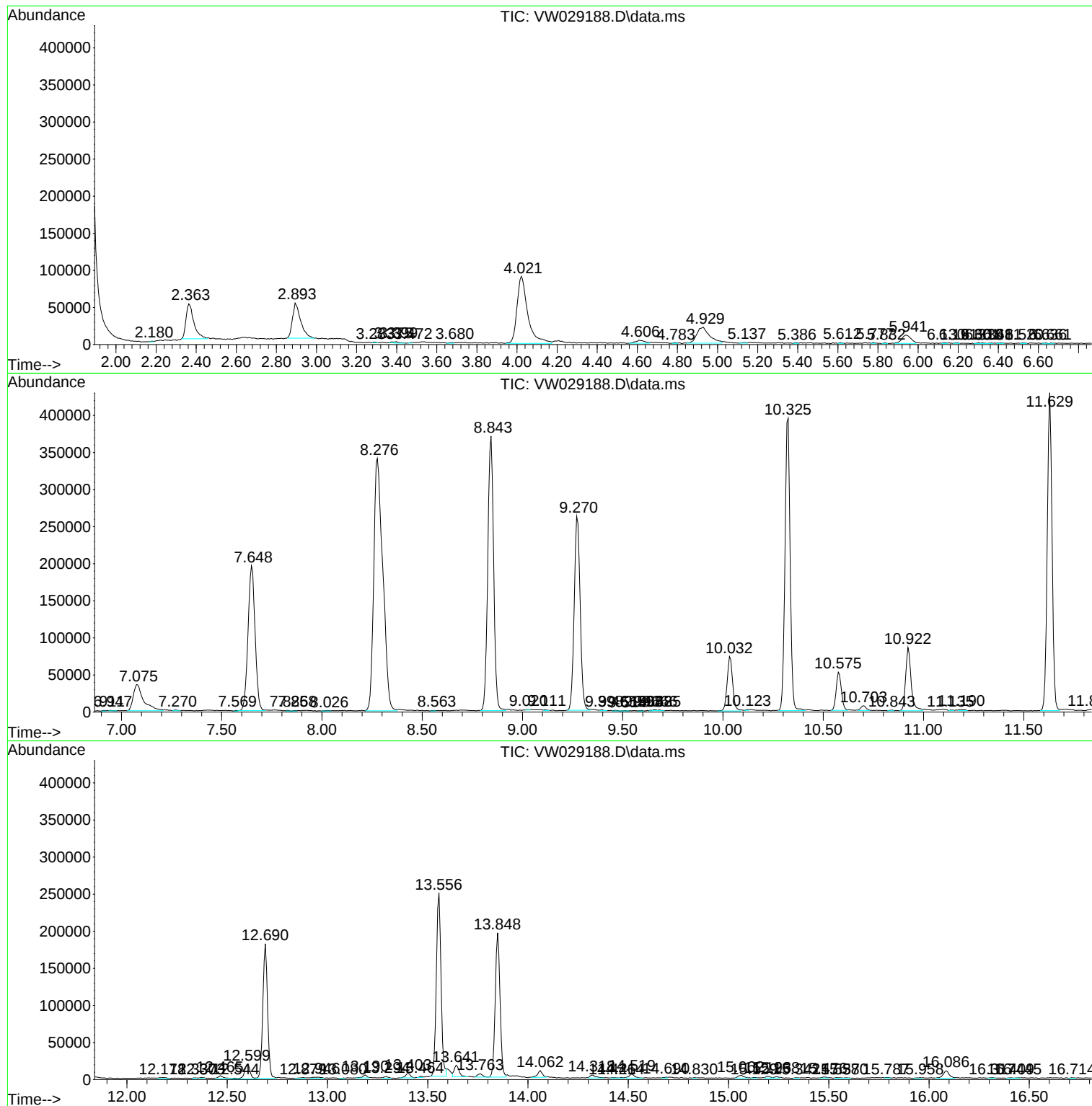
Sum of corrected areas: 6776662

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM061824SMA.M
Quant Title : SFAM01.0

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



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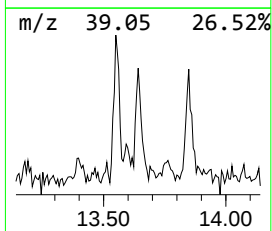
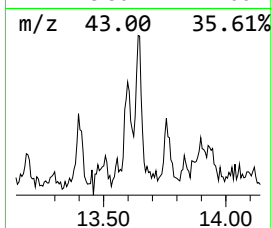
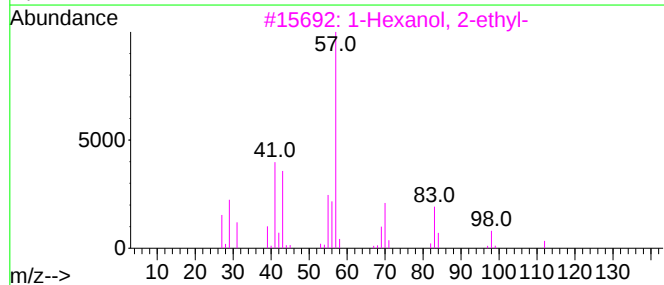
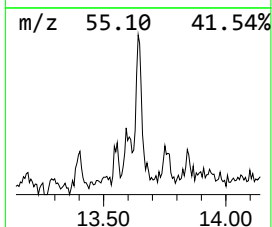
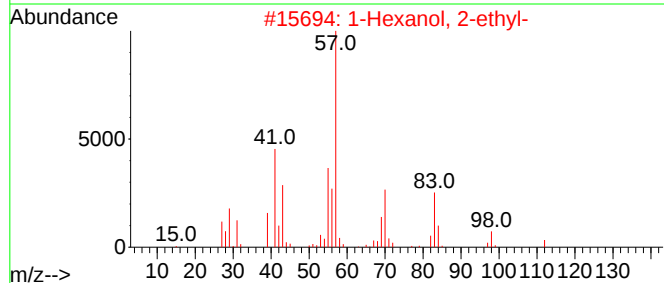
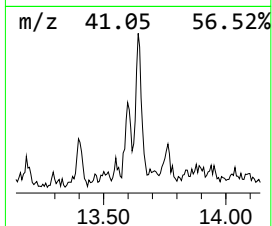
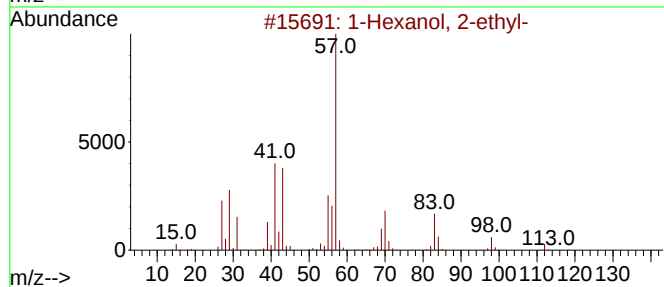
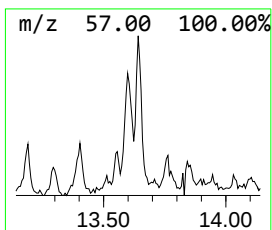
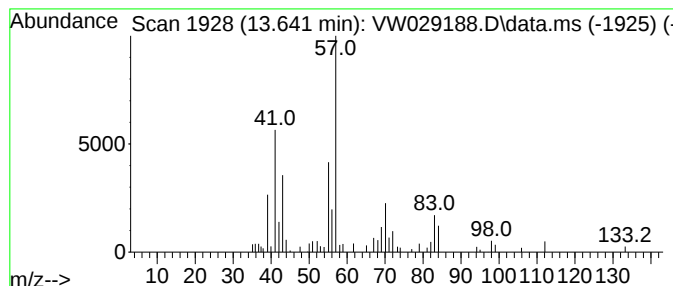
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM061824SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.641	1.62 ug/L	26071	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	64
4	Octane, 2,3-dimethyl-			142	C10H22	007146-60-3	50
5	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	50



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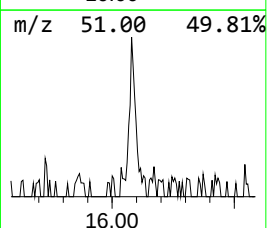
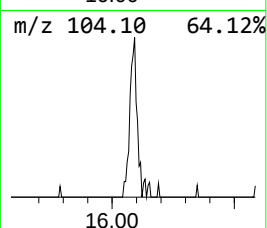
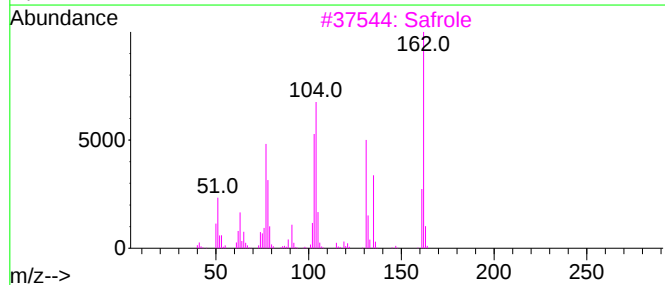
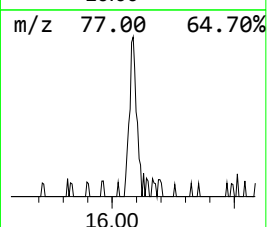
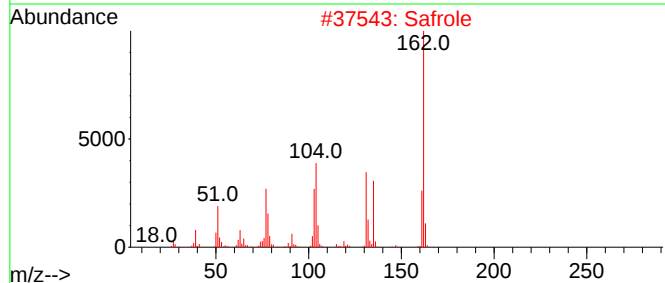
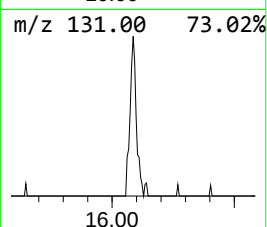
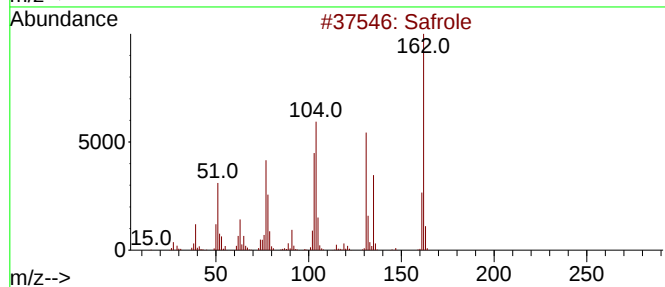
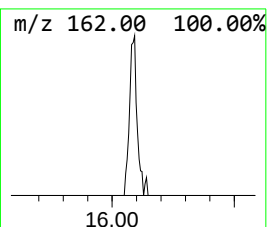
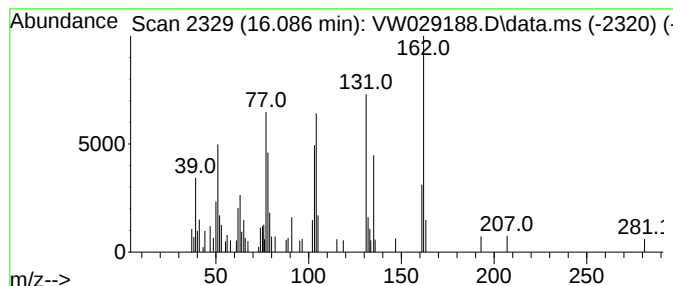
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM061824SMA.M
Quant Title : SFAM01.0

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

Peak Number 4 Safrole Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.086	1.34 ug/L	21609	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Safrole	162	C10H10O2	000094-59-7	95
2			Safrole	162	C10H10O2	000094-59-7	94
3			Safrole	162	C10H10O2	000094-59-7	94
4			Benzene, 1,2-(methylenedioxy)-4-...	162	C10H10O2	004043-71-4	93
5			1,3-Benzodioxole, 5-(1-propenyl)...	162	C10H10O2	017627-76-8	93



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Quant Title : SFAM01.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Hexanol, 2-et...	13.641	1.6	ug/L	26071	3	13.556	402609	25.0
Safrole	16.086	1.3	ug/L	21609	3	13.556	402609	25.0