

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012925\
 Data File : VX044764.D
 Acq On : 29 Jan 2025 12:57
 Operator : JC/MD
 Sample : Q1190-11ME
 Misc : 4.39g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A44T0ME

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_X\Method\SFAMXML012825WMA.M
 Title : VOC Analysis

Signal : TIC: VX044764.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	22	28	34	rBV2	10507	23176	2.16%	0.271%
2	1.368	42	46	49	rBV	90816	98864	9.20%	1.156%
3	1.563	72	78	79	rBV2	5407	8442	0.79%	0.099%
4	1.648	89	92	97	rBV	16200	21933	2.04%	0.256%
5	2.282	189	196	213	rBV	205755	340534	31.70%	3.982%
6	2.721	261	268	274	rVB2	2655	5616	0.52%	0.066%
7	2.837	283	287	295	rVB4	2576	5333	0.50%	0.062%
8	2.940	297	304	313	rBV2	2977	6873	0.64%	0.080%
9	3.142	334	337	339	rBV2	400	458	0.04%	0.005%
10	3.257	351	356	358	rBV2	208	411	0.04%	0.005%
11	3.428	375	384	391	rVB6	950	2856	0.27%	0.033%
12	3.562	405	406	409	rBV	335	422	0.04%	0.005%
13	4.001	473	478	482	rBV2	246	528	0.05%	0.006%
14	4.483	549	557	583	rBV2	42755	180746	16.83%	2.114%
15	4.904	625	626	629	rBV3	427	479	0.04%	0.006%
16	5.056	639	651	669	rBV	138772	430582	40.09%	5.035%
17	5.385	703	705	707	rBV	504	428	0.04%	0.005%
18	5.470	717	719	722	rVB2	556	543	0.05%	0.006%
19	5.562	725	734	738	rBV3	706	1950	0.18%	0.023%
20	5.958	788	799	816	rBV2	374924	1074159	100.00%	12.561%
21	6.403	870	872	877	rVB3	537	597	0.06%	0.007%
22	6.757	920	930	957	rBV	253848	634043	59.03%	7.414%
23	7.306	1011	1020	1037	rBV	226093	515778	48.02%	6.031%
24	7.482	1046	1049	1052	rBV3	720	855	0.08%	0.010%
25	7.696	1083	1084	1087	rBV2	442	473	0.04%	0.006%
26	7.976	1123	1130	1133	rBV4	1030	2149	0.20%	0.025%
27	8.007	1133	1135	1139	rVB3	766	984	0.09%	0.012%
28	8.061	1142	1144	1146	rVB2	566	452	0.04%	0.005%
29	8.086	1146	1148	1151	rBV3	377	600	0.06%	0.007%
30	8.257	1172	1176	1181	rVV2	4045	5699	0.53%	0.067%
31	8.324	1181	1187	1208	rVB	181360	316152	29.43%	3.697%
32	8.647	1233	1240	1266	rVV	608648	1046113	97.39%	12.233%
33	8.909	1280	1283	1284	rBV2	816	705	0.07%	0.008%
34	8.952	1284	1290	1303	rVV	119404	195617	18.21%	2.287%
35	9.275	1338	1343	1347	rVB3	3391	5234	0.49%	0.061%
36	9.391	1357	1362	1384	rBV	245621	441666	41.12%	5.165%

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 ClientSampleId :
 A44T0ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012825WMA.M
 Title : VOC Analysis

37	9.634	1401	1402	1405	rBV2	524	437	0.04%	0.005%
38	9.708	1411	1414	1418	rBV3	1555	2676	0.25%	0.031%
39	9.896	1443	1445	1449	rVV3	417	565	0.05%	0.007%
40	10.049	1465	1470	1488	rBV	550955	835292	77.76%	9.768%
41	10.354	1518	1520	1528	rVB4	1134	2010	0.19%	0.024%
42	10.427	1528	1532	1533	rVB2	508	511	0.05%	0.006%
43	10.451	1533	1536	1539	rBV	371	622	0.06%	0.007%
44	10.610	1560	1562	1564	rBV	377	413	0.04%	0.005%
45	10.646	1566	1568	1572	rVB2	535	633	0.06%	0.007%
46	10.781	1587	1590	1591	rVB	614	489	0.05%	0.006%
47	10.817	1591	1596	1598	rBV2	668	1062	0.10%	0.012%
48	10.939	1613	1616	1619	rBV3	583	881	0.08%	0.010%
49	11.079	1635	1639	1640	rBV2	448	539	0.05%	0.006%
50	11.189	1652	1657	1670	rBV	419991	573895	53.43%	6.711%
51	11.311	1673	1677	1682	rVB4	1796	2670	0.25%	0.031%
52	11.439	1696	1698	1700	rBV2	522	696	0.06%	0.008%
53	11.476	1700	1704	1710	rVB4	2454	3878	0.36%	0.045%
54	11.610	1723	1726	1729	rBV2	484	473	0.04%	0.006%
55	11.683	1731	1738	1739	rBV3	857	1272	0.12%	0.015%
56	11.744	1746	1748	1753	rVB3	1345	1673	0.16%	0.020%
57	11.872	1766	1769	1772	rBV2	586	640	0.06%	0.007%
58	11.933	1775	1779	1782	rBV2	1184	1577	0.15%	0.018%
59	11.975	1783	1786	1788	rVB3	922	808	0.08%	0.009%
60	12.018	1788	1793	1805	rBV	589816	763650	71.09%	8.930%
61	12.189	1820	1821	1824	rVB2	564	402	0.04%	0.005%
62	12.317	1837	1842	1856	rBV	653257	838361	78.05%	9.804%
63	12.420	1856	1859	1864	rVB4	3896	4989	0.46%	0.058%
64	12.579	1881	1885	1886	rBV3	682	701	0.07%	0.008%
65	12.762	1911	1915	1918	rVB2	2791	3515	0.33%	0.041%
66	12.884	1930	1935	1939	rBV6	920	1905	0.18%	0.022%
67	12.975	1948	1950	1953	rVB	675	623	0.06%	0.007%
68	13.048	1960	1962	1965	rVV3	720	653	0.06%	0.008%
69	13.134	1972	1976	1978	rVB2	469	531	0.05%	0.006%
70	13.183	1983	1984	1986	rBV2	521	408	0.04%	0.005%
71	13.268	1994	1998	2004	rVB2	4488	6078	0.57%	0.071%
72	13.317	2004	2006	2009	rVB2	521	476	0.04%	0.006%
73	13.384	2011	2017	2018	rBV2	1044	1577	0.15%	0.018%
74	13.512	2036	2038	2041	rVB2	674	573	0.05%	0.007%
75	13.536	2041	2042	2045	rBV3	480	445	0.04%	0.005%
76	13.689	2063	2067	2070	rBV3	937	1334	0.12%	0.016%

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 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A44TOME

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_X\Method\SFAMXML012825WMA.M
 Title : VOC Analysis

77	13.786	2078	2083	2088	rVB	3787	5662	0.53%	0.066%
78	13.969	2108	2113	2115	rBV3	528	807	0.08%	0.009%
79	14.036	2119	2124	2129	rVV	5228	6888	0.64%	0.081%
80	14.127	2136	2139	2144	rVB3	1808	2714	0.25%	0.032%
81	14.432	2185	2189	2199	rBV	43657	62173	5.79%	0.727%
82	14.609	2216	2218	2219	rBV	940	636	0.06%	0.007%
83	14.640	2220	2223	2231	rVV5	1897	3629	0.34%	0.042%
84	14.755	2238	2242	2244	rVV3	3479	4656	0.43%	0.054%
85	14.786	2244	2247	2255	rVB4	3725	5282	0.49%	0.062%
86	15.213	2315	2317	2323	rVB4	1436	1966	0.18%	0.023%
87	15.396	2344	2347	2348	rBV3	973	1054	0.10%	0.012%
88	15.487	2357	2362	2367	rBV7	3163	5952	0.55%	0.070%
89	15.615	2379	2383	2387	rBV5	3234	5358	0.50%	0.063%
90	15.798	2411	2413	2414	rBV2	1013	720	0.07%	0.008%
91	15.859	2418	2423	2427	rVB5	2824	4434	0.41%	0.052%
92	15.956	2434	2439	2440	rBV4	640	1015	0.09%	0.012%
93	16.084	2458	2460	2464	rBV4	933	1228	0.11%	0.014%
94	16.115	2464	2465	2467	rVB	936	487	0.05%	0.006%
95	16.261	2486	2489	2490	rBV2	777	596	0.06%	0.007%
96	16.322	2497	2499	2504	rBV3	1052	1362	0.13%	0.016%
97	16.365	2504	2506	2507	rBV2	474	414	0.04%	0.005%
98	16.426	2515	2516	2518	rBV2	542	429	0.04%	0.005%
99	16.664	2550	2555	2558	rBV5	1402	2200	0.20%	0.026%
100	16.731	2565	2566	2569	rVB3	729	583	0.05%	0.007%

Sum of corrected areas: 8551628

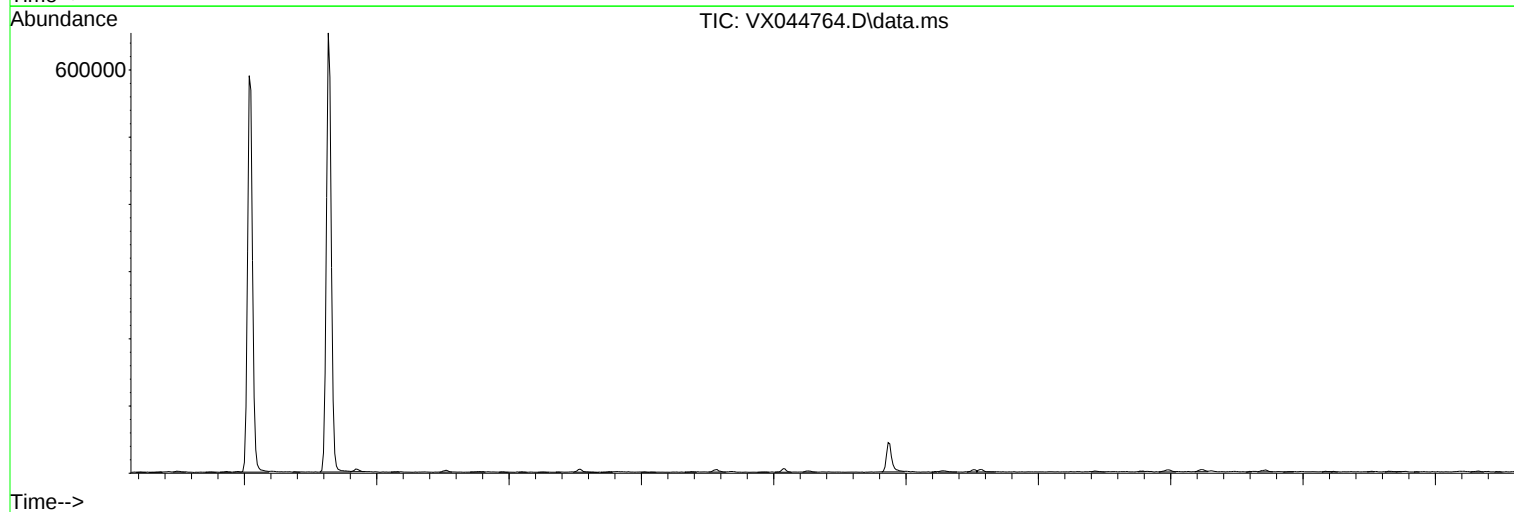
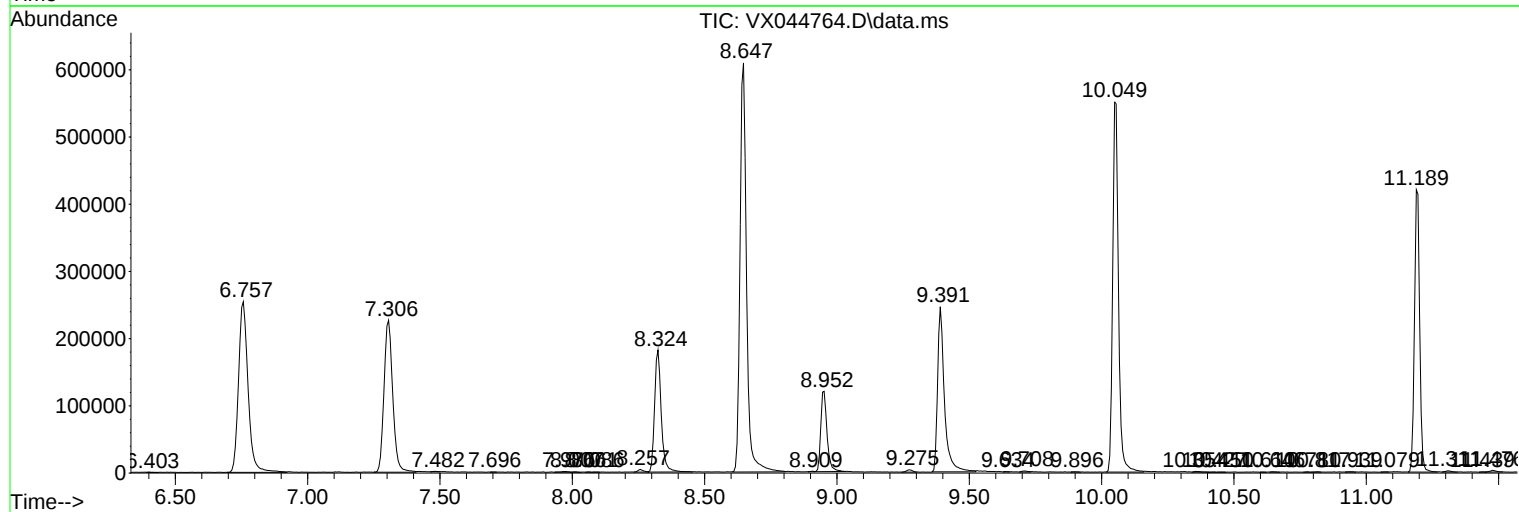
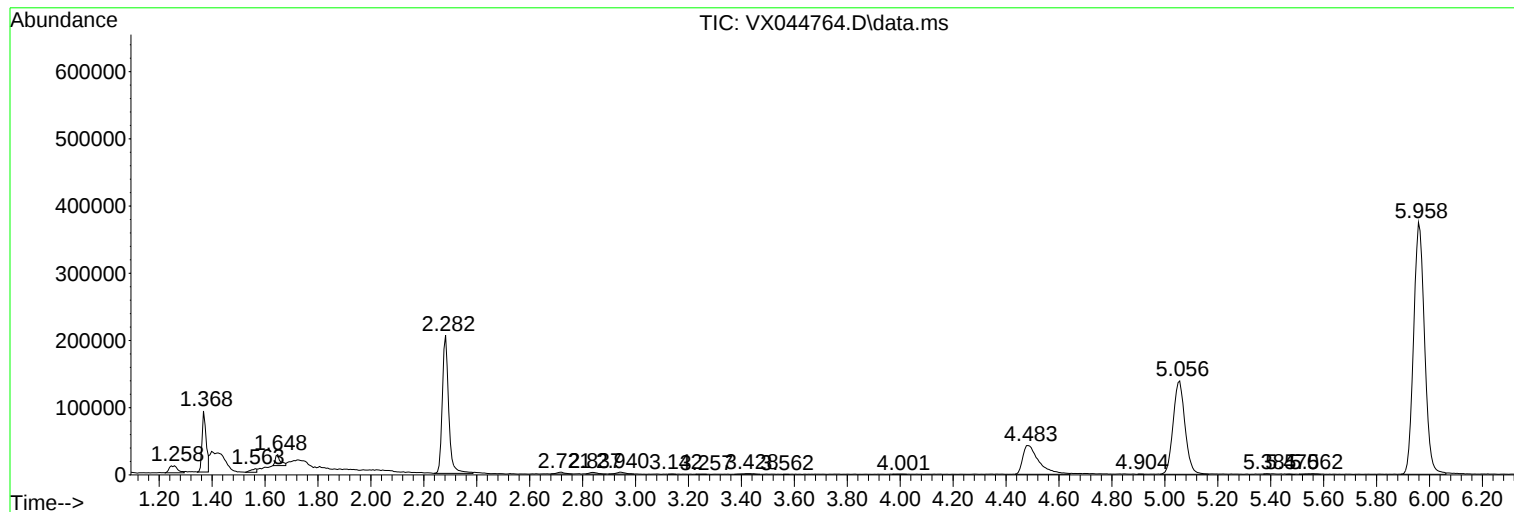
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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44T0ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012825WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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Instrument :
MSVOA_X
ClientSampleId :
A44T0ME

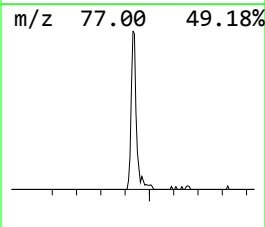
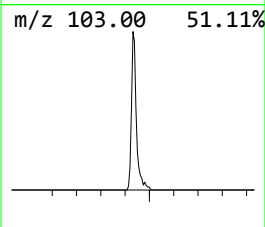
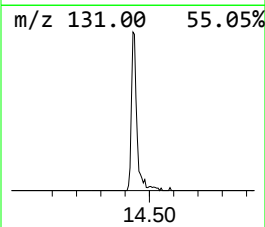
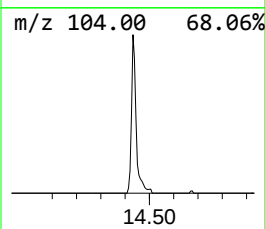
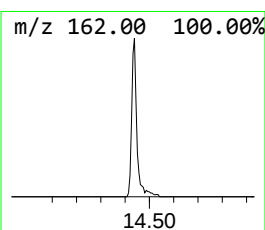
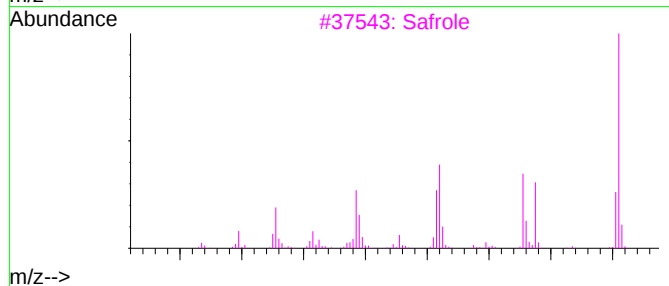
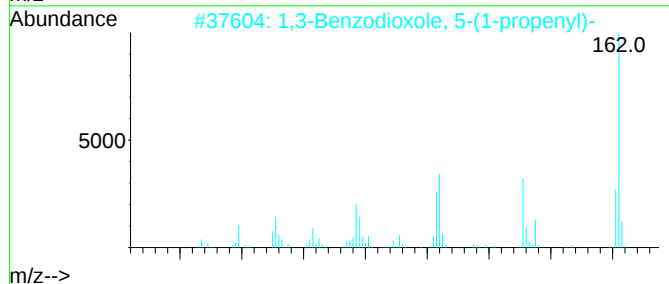
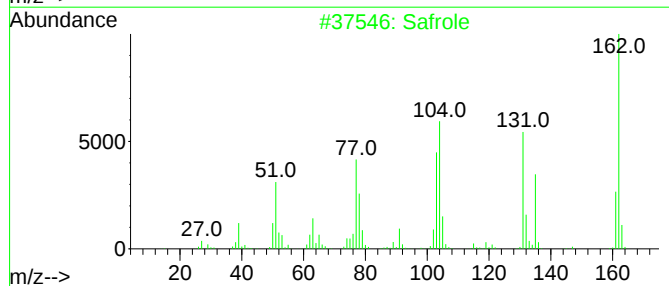
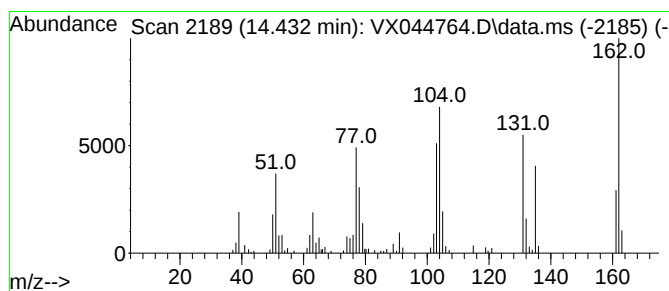
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM012825WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 2 Safole Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.432	4.07 ug/L	62173	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Safole	162	C10H10O2	000094-59-7	98
2	1,3-Benzodioxole, 5-(1-propenyl)-	162	C10H10O2	000120-58-1	97
3	Safole	162	C10H10O2	000094-59-7	97
4	1,3-Benzodioxole, 5-(1-propenyl)...	162	C10H10O2	017627-76-8	97
5	1,3-Benzodioxole, 5-(1-propenyl)-	162	C10H10O2	000120-58-1	97



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Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Safrole	14.432	4.1	ug/L	62173	3	12.024	763650	50.0