

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV111323\
 Data File : VV032947.D
 Acq On : 13 Nov 2023 21:39
 Operator : SY/MD
 Sample : 05296-19 4X
 Misc : 5.89gm/5mL/100uL/5mL/MSVOA_V/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BH3T7

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_V\Method\SFAMVLM111323WMA.M
 Title : VOC Analysis

Signal : TIC: VV032947.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.278	67	74	88	rBV	284428	309108	10.37%	1.514%
2	1.468	109	133	134	rBV3	47645	142812	4.79%	0.700%
3	1.513	141	147	165	rVB	236464	306770	10.29%	1.503%
4	2.053	305	315	331	rBV	524467	763976	25.62%	3.742%
5	2.208	360	363	364	rBV3	1973	1106	0.04%	0.005%
6	2.278	382	385	391	rVB8	1579	1204	0.04%	0.006%
7	2.339	402	404	407	rVB4	1679	1061	0.04%	0.005%
8	2.365	407	412	413	rBV5	1191	824	0.03%	0.004%
9	2.388	413	419	422	rBV7	2580	3192	0.11%	0.016%
10	2.558	462	472	480	rVV3	9327	20215	0.68%	0.099%
11	2.690	506	513	514	rBV7	2102	1889	0.06%	0.009%
12	2.796	542	546	549	rVB6	1729	1195	0.04%	0.006%
13	2.947	589	593	595	rBV5	1747	1244	0.04%	0.006%
14	3.015	611	614	616	rVV4	1531	943	0.03%	0.005%
15	3.037	616	621	624	rVV6	1695	1878	0.06%	0.009%
16	3.066	628	630	637	rVV6	1820	1487	0.05%	0.007%
17	3.095	637	639	642	rVV4	1989	1040	0.03%	0.005%
18	3.256	687	689	692	rVV4	1457	921	0.03%	0.005%
19	3.278	692	696	701	rVB7	1704	1692	0.06%	0.008%
20	3.301	701	703	705	rBV3	1499	994	0.03%	0.005%
21	3.336	711	714	718	rBV4	1348	920	0.03%	0.005%
22	3.365	718	723	727	rVV8	1683	1622	0.05%	0.008%
23	3.388	727	730	733	rVV5	1054	857	0.03%	0.004%
24	3.400	733	734	739	rVB5	1247	857	0.03%	0.004%
25	3.426	739	742	745	rBV5	1639	1181	0.04%	0.006%
26	3.445	745	748	751	rVV5	1627	1109	0.04%	0.005%
27	3.490	760	762	765	rVB4	1483	821	0.03%	0.004%
28	3.545	776	779	782	rVB5	1402	991	0.03%	0.005%
29	3.571	784	787	792	rBV5	1434	1733	0.06%	0.008%
30	3.625	800	804	806	rBV5	1605	1166	0.04%	0.006%
31	3.744	836	841	844	rBV5	1639	1675	0.06%	0.008%
32	3.783	844	853	887	rBV	100353	286895	9.62%	1.405%
33	4.021	926	927	931	rVB3	1514	903	0.03%	0.004%
34	4.169	969	973	976	rBV6	1793	1809	0.06%	0.009%
35	4.246	981	997	1027	rVV	318516	813334	27.27%	3.984%
36	4.564	1093	1096	1100	rBV5	1679	1360	0.05%	0.007%

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 Title : VOC Analysis

37	4.664	1124	1127	1130	rVV5	1664	1261	0.04%	0.006%
38	4.703	1136	1139	1143	rBV6	1411	1179	0.04%	0.006%
39	4.860	1186	1188	1196	rVB9	2576	2086	0.07%	0.010%
40	4.953	1196	1217	1249	rBV2	755029	1981311	66.44%	9.705%
41	5.188	1287	1290	1292	rBV4	1203	868	0.03%	0.004%
42	5.333	1330	1335	1339	rBV8	2120	2206	0.07%	0.011%
43	5.410	1356	1359	1365	rVV6	1838	1977	0.07%	0.010%
44	5.532	1385	1397	1426	rBV	540263	1109289	37.20%	5.434%
45	5.937	1519	1523	1525	rBV5	1517	1237	0.04%	0.006%
46	5.986	1526	1538	1569	rVV	424708	870604	29.20%	4.264%
47	6.278	1627	1629	1632	rVB2	1633	824	0.03%	0.004%
48	6.307	1635	1638	1640	rVV4	2099	1584	0.05%	0.008%
49	6.342	1646	1649	1651	rVV4	1316	843	0.03%	0.004%
50	6.381	1659	1661	1667	rVB7	2967	2105	0.07%	0.010%
51	6.452	1681	1683	1689	rVB5	1755	1624	0.05%	0.008%
52	6.481	1689	1692	1695	rBV5	1773	1564	0.05%	0.008%
53	6.802	1788	1792	1797	rVB8	1758	1587	0.05%	0.008%
54	6.873	1812	1814	1816	rBV3	1398	869	0.03%	0.004%
55	6.912	1816	1826	1844	rVV	240933	438873	14.72%	2.150%
56	7.146	1896	1899	1901	rBV3	1006	865	0.03%	0.004%
57	7.243	1918	1929	1950	rBV	923934	1593521	53.44%	7.806%
58	7.439	1987	1990	1993	rBV5	1739	1311	0.04%	0.006%
59	7.551	2016	2025	2045	rBV	172000	314723	10.55%	1.542%
60	7.770	2089	2093	2094	rBV3	1738	1200	0.04%	0.006%
61	7.809	2100	2105	2107	rBV5	1905	1762	0.06%	0.009%
62	7.850	2114	2118	2121	rBV6	2532	1816	0.06%	0.009%
63	7.870	2122	2124	2126	rBV3	1634	859	0.03%	0.004%
64	7.976	2153	2157	2158	rBV3	1607	960	0.03%	0.005%
65	8.027	2163	2173	2198	rVV	421633	755197	25.32%	3.699%
66	8.281	2245	2252	2253	rBV5	5509	6008	0.20%	0.029%
67	8.368	2274	2279	2284	rBV9	3806	4412	0.15%	0.022%
68	8.445	2299	2303	2306	rBV6	2450	1996	0.07%	0.010%
69	8.487	2312	2316	2318	rBV5	1402	1236	0.04%	0.006%
70	8.645	2362	2365	2368	rBV5	1576	1264	0.04%	0.006%
71	8.709	2380	2385	2386	rBV5	2855	2107	0.07%	0.010%
72	8.786	2398	2409	2438	rBV	868191	1466055	49.16%	7.181%
73	8.992	2471	2473	2474	rBV2	2595	1119	0.04%	0.005%
74	9.088	2497	2503	2513	rVB7	9622	14469	0.49%	0.071%
75	9.194	2535	2536	2541	rVB5	1810	1070	0.04%	0.005%
76	9.249	2551	2553	2561	rVB7	3196	3530	0.12%	0.017%

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 Title : VOC Analysis

77	9.288	2561	2565	2567	rBV5	1300	837	0.03%	0.004%
78	9.352	2580	2585	2587	rBV6	2120	1854	0.06%	0.009%
79	9.371	2587	2591	2592	rBV4	2360	1382	0.05%	0.007%
80	9.448	2613	2615	2620	rVB5	2382	1572	0.05%	0.008%
81	9.487	2624	2627	2628	rBV3	3539	1994	0.07%	0.010%
82	9.561	2647	2650	2651	rBV3	1658	923	0.03%	0.005%
83	9.741	2699	2706	2712	rVB3	3140	4872	0.16%	0.024%
84	9.844	2730	2738	2746	rBV3	6918	12194	0.41%	0.060%
85	10.014	2784	2791	2795	rBV9	2128	3290	0.11%	0.016%
86	10.066	2803	2807	2817	rVB9	7909	10280	0.34%	0.050%
87	10.156	2820	2835	2857	rBV	668960	1061366	35.59%	5.199%
88	10.329	2875	2889	2898	rBV	64775	113666	3.81%	0.557%
89	10.442	2918	2924	2925	rBV4	4626	3269	0.11%	0.016%
90	10.477	2927	2935	2945	rVV2	59554	90740	3.04%	0.444%
91	10.940	3075	3079	3081	rBV5	1888	1267	0.04%	0.006%
92	10.969	3081	3088	3089	rBV6	8205	7518	0.25%	0.037%
93	11.117	3117	3134	3146	rBV	872448	1381037	46.31%	6.765%
94	11.188	3146	3156	3190	rVB2	1150386	2888621	96.87%	14.149%
95	11.564	3261	3273	3292	rBV2	1358095	2982031	100.00%	14.607%
96	12.310	3498	3505	3512	rBV6	23690	39942	1.34%	0.196%
97	12.410	3529	3536	3543	rBV4	38923	55513	1.86%	0.272%
98	12.506	3559	3566	3582	rVV	83712	157851	5.29%	0.773%
99	12.587	3585	3591	3602	rVB2	52012	82227	2.76%	0.403%
100	13.201	3774	3782	3800	rBV	148431	232860	7.81%	1.141%

Sum of corrected areas: 20415261

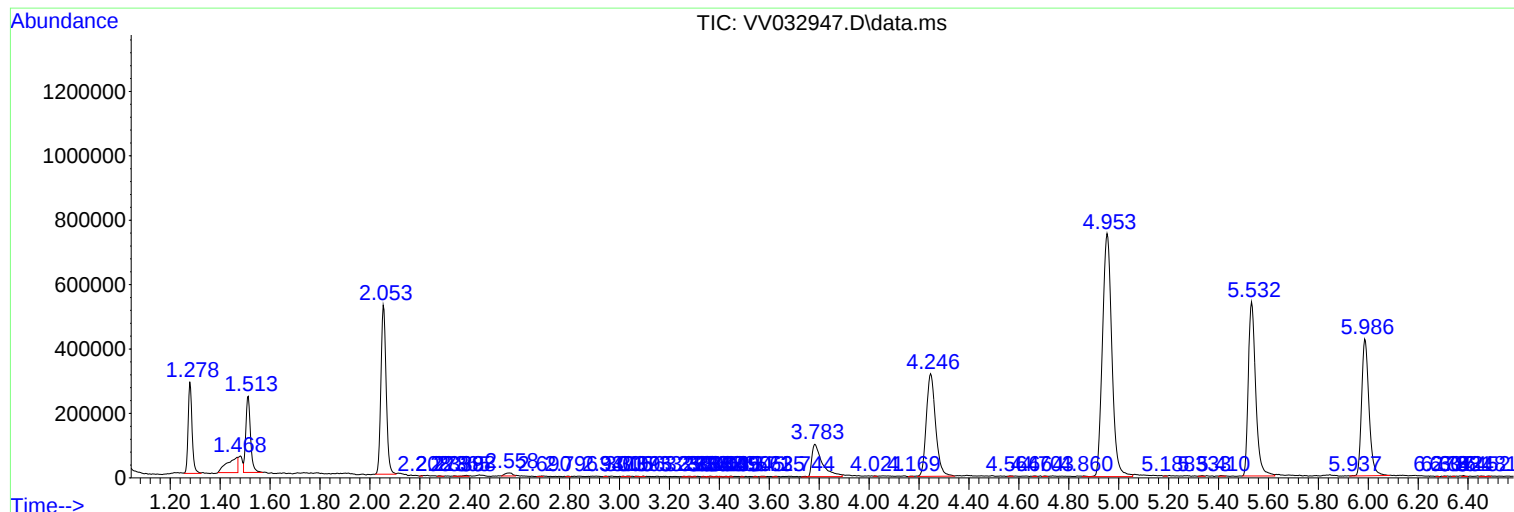
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM111323WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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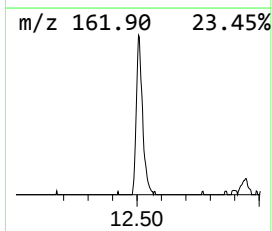
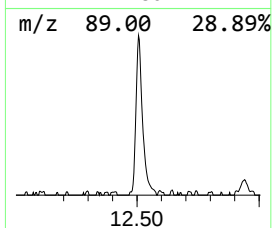
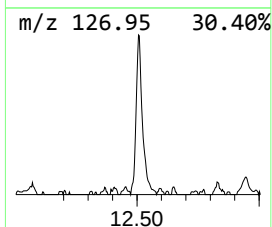
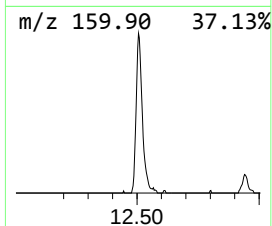
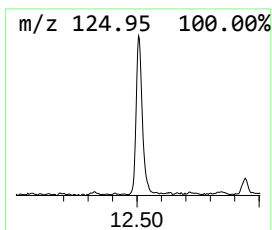
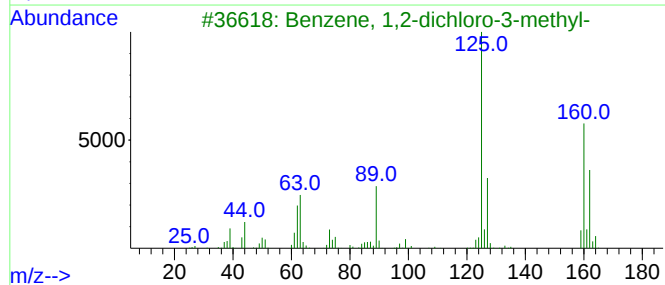
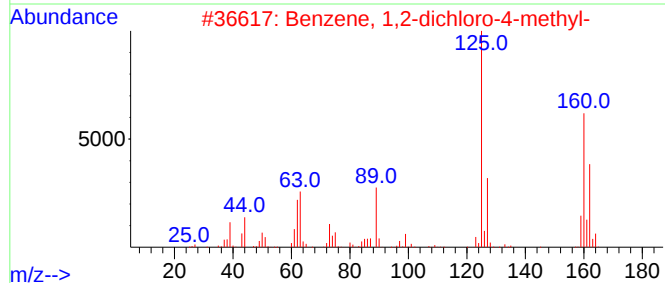
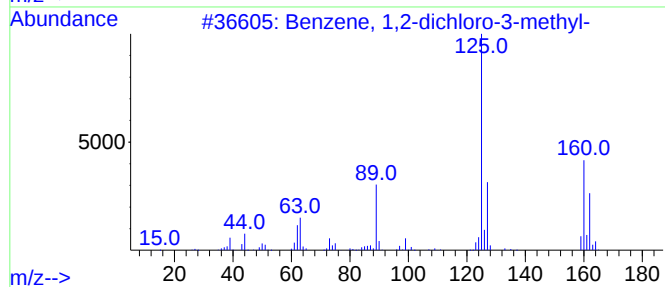
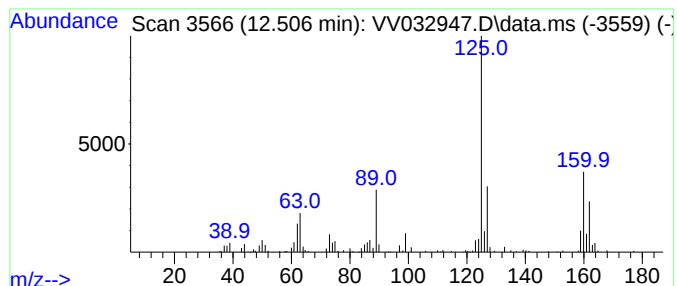
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM111323WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Benzene, 1,2-dichloro-3-met... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.506	2.73 ug/L	157851	1,4-Dichlorobenzene-d4	11.188

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2-dichloro-3-methyl-	160	C7H6Cl2	032768-54-0	98
2			Benzene, 1,2-dichloro-4-methyl-	160	C7H6Cl2	000095-75-0	97
3			Benzene, 1,2-dichloro-3-methyl-	160	C7H6Cl2	032768-54-0	97
4			Benzene, 1,2-dichloro-3-methyl-	160	C7H6Cl2	032768-54-0	97
5			Benzene, 1,3-dichloro-2-methyl-	160	C7H6Cl2	000118-69-4	96



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, 1,2-di...	12.506	2.7	ug/L	157851	3	11.188	2888620	50.0