

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121324\
 Data File : VX044304.D
 Acq On : 13 Dec 2024 23:58
 Operator : JC/MD
 Sample : P5153-05ME
 Misc : 7.21g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E28P3ME

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\SFAMXLM120524WMA.M
 Title : VOC Analysis

Signal : TIC: VX044304.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	26	29	37	rVB	11933	13453	1.72%	0.209%
2	1.368	43	46	48	rBV	35914	37936	4.84%	0.590%
3	1.581	70	81	82	rBV2	16915	46838	5.98%	0.728%
4	2.276	189	195	208	rBV	123188	205934	26.28%	3.202%
5	2.623	250	252	254	rBV2	504	523	0.07%	0.008%
6	2.940	297	304	315	rVB6	3593	9545	1.22%	0.148%
7	3.056	321	323	325	rBV2	1156	1210	0.15%	0.019%
8	3.209	346	348	352	rVB4	616	628	0.08%	0.010%
9	3.416	377	382	391	rVV3	4625	9893	1.26%	0.154%
10	4.160	498	504	505	rBV2	412	680	0.09%	0.011%
11	4.263	518	521	522	rBV2	2471	2276	0.29%	0.035%
12	4.495	550	559	580	rBV	28796	133451	17.03%	2.075%
13	5.056	638	651	666	rBV2	95765	318887	40.70%	4.958%
14	5.586	735	738	739	rBV3	643	681	0.09%	0.011%
15	5.787	767	771	772	rBV3	1012	1035	0.13%	0.016%
16	5.958	788	799	821	rBV2	274763	783565	100.00%	12.183%
17	6.336	856	861	865	rBV6	2618	4961	0.63%	0.077%
18	6.586	899	902	904	rBV3	455	687	0.09%	0.011%
19	6.751	921	929	947	rVV	212749	529361	67.56%	8.231%
20	7.123	982	990	991	rBV6	2001	4299	0.55%	0.067%
21	7.299	1012	1019	1027	rBV2	157500	361296	46.11%	5.617%
22	7.482	1046	1049	1050	rBV2	870	946	0.12%	0.015%
23	7.586	1065	1066	1070	rBV2	603	662	0.08%	0.010%
24	7.641	1072	1075	1078	rBV4	1156	1751	0.22%	0.027%
25	7.763	1092	1095	1099	rVB4	1482	2224	0.28%	0.035%
26	7.952	1121	1126	1131	rVB6	1843	3914	0.50%	0.061%
27	8.074	1144	1146	1149	rVB3	719	633	0.08%	0.010%
28	8.104	1149	1151	1155	rBV3	536	769	0.10%	0.012%
29	8.269	1172	1178	1181	rBV4	1816	3116	0.40%	0.048%
30	8.324	1181	1187	1199	rVV	80769	147663	18.85%	2.296%
31	8.506	1215	1217	1221	rBV4	743	1107	0.14%	0.017%
32	8.543	1221	1223	1226	rVB4	488	617	0.08%	0.010%
33	8.592	1226	1231	1232	rBV3	2773	3775	0.48%	0.059%
34	8.647	1234	1240	1248	rVV	363155	588620	75.12%	9.152%
35	8.714	1249	1251	1258	rVB	8667	13529	1.73%	0.210%
36	8.909	1279	1283	1285	rBV4	2305	3042	0.39%	0.047%

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 Title : VOC Analysis

37	8.952	1285	1290	1303	rVB	59370	96850	12.36%	1.506%
38	9.201	1328	1331	1334	rBV3	841	853	0.11%	0.013%
39	9.281	1341	1344	1346	rBV	1032	1197	0.15%	0.019%
40	9.390	1357	1362	1377	rBV	134711	306887	39.17%	4.772%
41	9.555	1386	1389	1395	rVB2	4611	6007	0.77%	0.093%
42	9.616	1395	1399	1402	rBV3	4653	6576	0.84%	0.102%
43	9.750	1419	1421	1422	rBV	783	717	0.09%	0.011%
44	9.817	1425	1432	1437	rBV5	3731	6500	0.83%	0.101%
45	9.896	1442	1445	1449	rBV3	1425	1739	0.22%	0.027%
46	9.964	1453	1456	1458	rBV2	579	807	0.10%	0.013%
47	10.006	1460	1463	1465	rBV3	1039	1095	0.14%	0.017%
48	10.055	1465	1471	1478	rBV	430853	631445	80.59%	9.818%
49	10.195	1491	1494	1501	rVB2	4084	6095	0.78%	0.095%
50	10.299	1503	1511	1517	rVV	16683	28211	3.60%	0.439%
51	10.354	1518	1520	1526	rVB5	4614	6254	0.80%	0.097%
52	10.579	1553	1557	1561	rBV5	1791	2274	0.29%	0.035%
53	10.640	1561	1567	1576	rVV	17108	25114	3.21%	0.390%
54	10.750	1581	1585	1587	rVV4	2075	2913	0.37%	0.045%
55	10.774	1587	1589	1594	rVB5	4698	5594	0.71%	0.087%
56	10.823	1594	1597	1598	rBV2	608	737	0.09%	0.011%
57	10.854	1598	1602	1605	rVV6	2003	3158	0.40%	0.049%
58	10.890	1606	1608	1613	rVB2	3245	3943	0.50%	0.061%
59	10.963	1617	1620	1626	rVV2	3106	3885	0.50%	0.060%
60	11.073	1636	1638	1639	rBV	1042	650	0.08%	0.010%
61	11.195	1652	1658	1669	rBV	265152	358979	45.81%	5.581%
62	11.305	1672	1676	1679	rBV3	3015	4293	0.55%	0.067%
63	11.384	1685	1689	1695	rVB4	5408	8878	1.13%	0.138%
64	11.451	1695	1700	1701	rBV2	3249	3887	0.50%	0.060%
65	11.475	1701	1704	1708	rVB2	5968	7325	0.93%	0.114%
66	11.610	1722	1726	1734	rVV2	5214	7948	1.01%	0.124%
67	11.677	1734	1737	1739	rVV4	690	743	0.09%	0.012%
68	11.713	1739	1743	1746	rVV2	4660	6025	0.77%	0.094%
69	11.750	1746	1749	1755	rVV	14792	20325	2.59%	0.316%
70	12.018	1788	1793	1800	rBV	452265	578390	73.82%	8.993%
71	12.085	1801	1804	1810	rVB	8906	13587	1.73%	0.211%
72	12.244	1826	1830	1834	rBV2	4884	7205	0.92%	0.112%
73	12.317	1837	1842	1853	rVV	420202	545352	69.60%	8.479%
74	12.420	1856	1859	1864	rVB2	9213	10901	1.39%	0.169%
75	12.530	1874	1877	1879	rBV4	2583	3468	0.44%	0.054%
76	12.609	1889	1890	1892	rBV2	917	577	0.07%	0.009%

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Integration Parameters: LSCINT.P

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Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
 Title : VOC Analysis

77	12.768	1913	1916	1919	rVB3	1507	2142	0.27%	0.033%
78	12.792	1919	1920	1922	rBV2	1008	701	0.09%	0.011%
79	12.969	1945	1949	1954	rBV5	3495	5020	0.64%	0.078%
80	13.134	1975	1976	1978	rBV2	820	657	0.08%	0.010%
81	13.262	1994	1997	2000	rBV3	6837	9299	1.19%	0.145%
82	13.378	2013	2016	2020	rBV4	3523	4772	0.61%	0.074%
83	13.579	2045	2049	2054	rBV5	3041	4300	0.55%	0.067%
84	13.774	2076	2081	2089	rVV	87166	111601	14.24%	1.735%
85	13.841	2089	2092	2095	rVB4	4209	5314	0.68%	0.083%
86	14.036	2120	2124	2128	rBV3	6015	7886	1.01%	0.123%
87	14.097	2132	2134	2140	rVV7	1538	2048	0.26%	0.032%
88	14.213	2150	2153	2155	rBV3	1207	1487	0.19%	0.023%
89	14.304	2166	2168	2169	rBV2	732	616	0.08%	0.010%
90	14.633	2215	2222	2233	rBV	50150	70577	9.01%	1.097%
91	14.780	2239	2246	2254	rVB	36827	54865	7.00%	0.853%
92	15.017	2283	2285	2288	rBV3	1058	1070	0.14%	0.017%
93	15.206	2313	2316	2321	rVB4	9917	13326	1.70%	0.207%
94	15.371	2339	2343	2347	rBV5	6595	11738	1.50%	0.183%
95	15.481	2356	2361	2367	rVB3	11632	21150	2.70%	0.329%
96	15.615	2378	2383	2386	rBV2	14947	24653	3.15%	0.383%
97	15.719	2398	2400	2402	rBV3	1838	1470	0.19%	0.023%
98	15.834	2412	2419	2428	rBV8	6515	17582	2.24%	0.273%
99	16.084	2457	2460	2467	rBV7	2798	5523	0.70%	0.086%
100	16.322	2493	2499	2512	rVB2	42873	86931	11.09%	1.352%

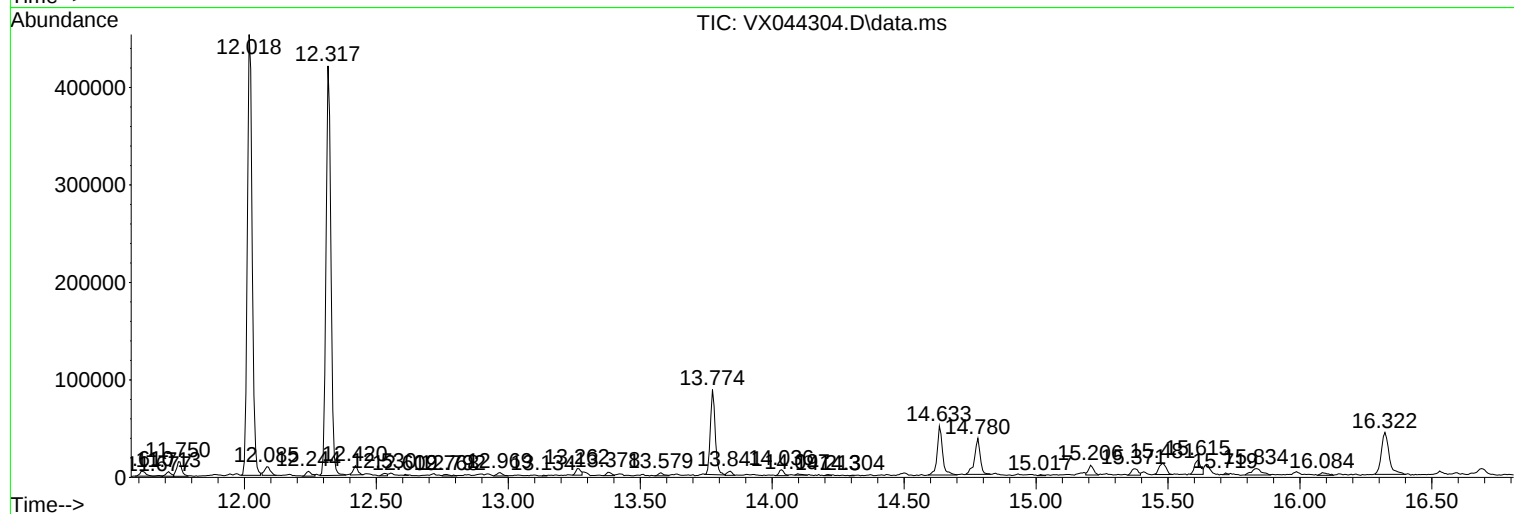
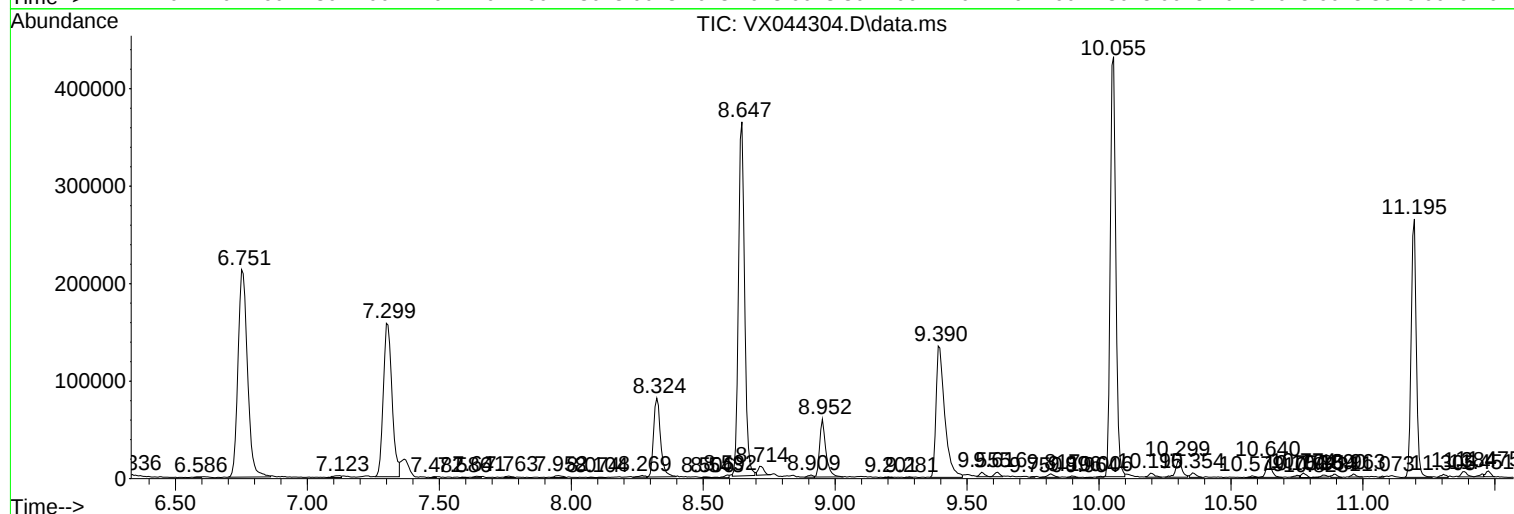
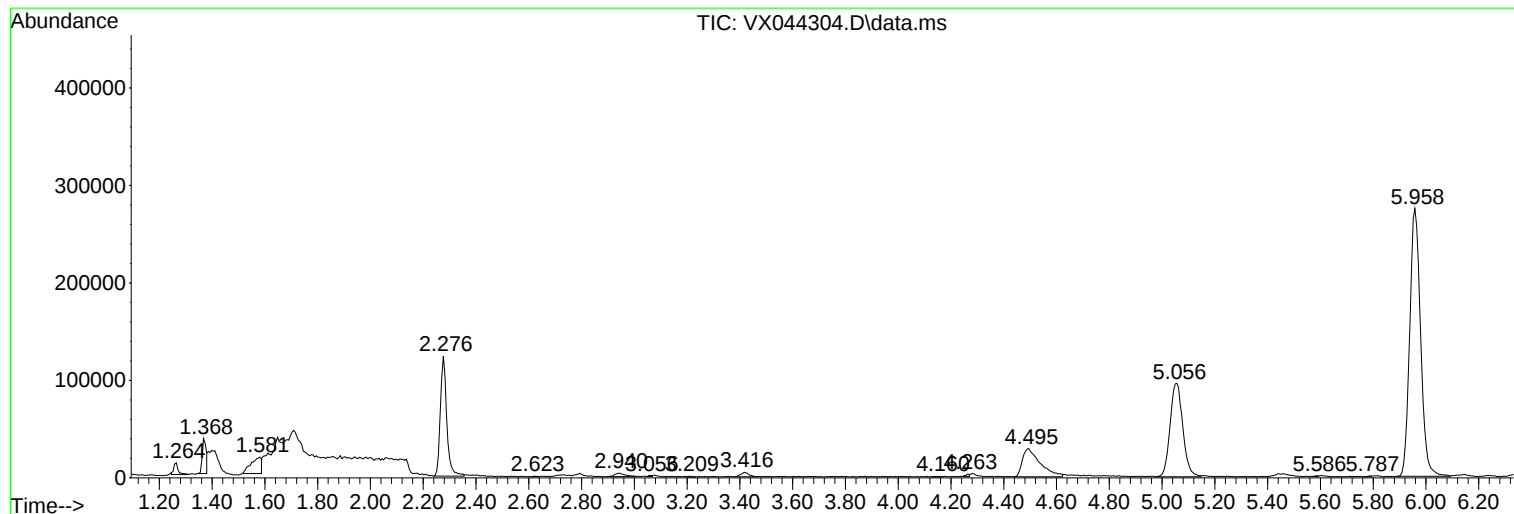
Sum of corrected areas: 6431619

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ALS Vial : 39 Sample Multiplier: 1

Instrument :
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ClientSampleId :
E28P3ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120524WMA.M
Quant Title : VOC Analysis

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



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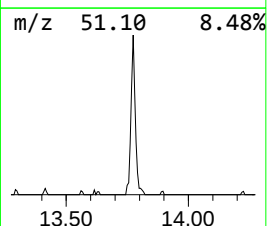
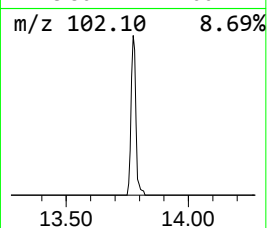
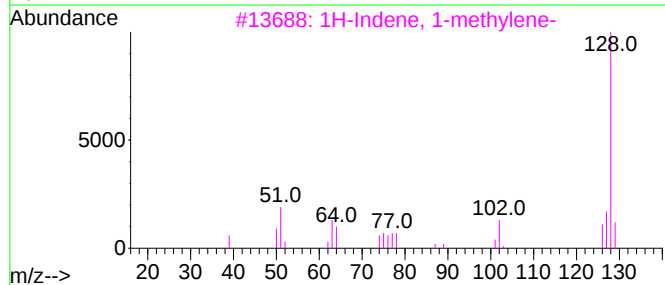
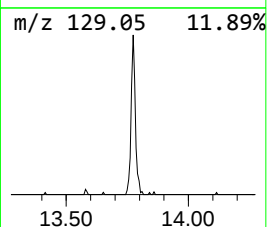
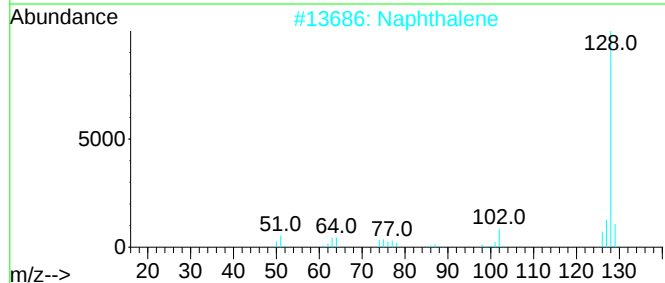
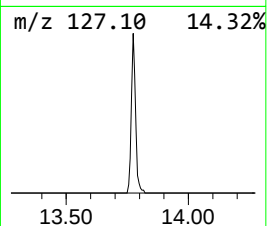
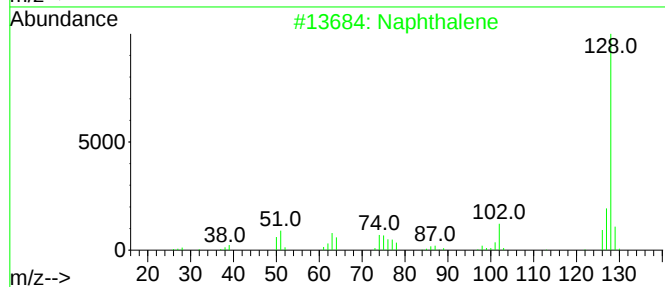
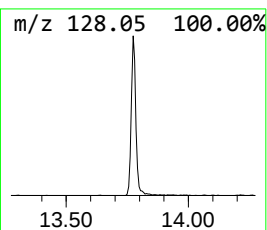
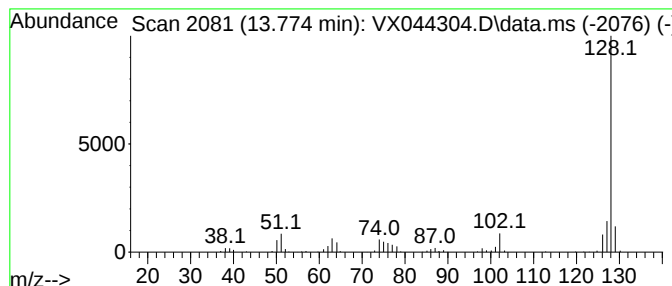
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 1H-Indene, 1-methylene- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	9.65 ug/L	111601	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	97
2			Naphthalene	128	C10H8	000091-20-3	95
3			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	94
4			Azulene	128	C10H8	000275-51-4	91
5			Azulene	128	C10H8	000275-51-4	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1H-Indene, 1-me...	13.774	9.7	ug/L	111601	3	12.018	578390	50.0