

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042623\
 Data File : VX035318.D
 Acq On : 26 Apr 2023 17:07
 Operator : JC/MD
 Sample : 02479-15ME
 Misc : 4.63g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EW974ME

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\SFAMXML041823WMA.M
 Title : VOC Analysis

Signal : TIC: VX035318.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	25	29	32	rBV2	2632	2927	0.21%	0.026%
2	1.367	42	46	51	rBV	66153	91487	6.54%	0.817%
3	1.672	88	96	100	rBV	31333	53791	3.84%	0.480%
4	2.288	191	197	212	rBV	250328	401318	28.67%	3.584%
5	2.715	261	267	273	rBV2	3307	6724	0.48%	0.060%
6	2.782	273	278	286	rVV6	3100	6564	0.47%	0.059%
7	3.434	373	385	390	rBV5	1364	3048	0.22%	0.027%
8	4.483	546	557	573	rBV	75030	266312	19.03%	2.378%
9	5.056	639	651	668	rBV	167797	536049	38.30%	4.787%
10	5.306	686	692	695	rBV5	1199	2502	0.18%	0.022%
11	5.550	723	732	738	rBV4	2325	5514	0.39%	0.049%
12	5.964	789	800	816	rBV2	490169	1399768	100.00%	12.501%
13	6.147	826	830	835	rVB4	944	1613	0.12%	0.014%
14	6.360	856	865	866	rBV3	3815	6593	0.47%	0.059%
15	6.757	921	930	949	rBV	414732	996679	71.20%	8.901%
16	7.007	967	971	974	rBV4	997	1593	0.11%	0.014%
17	7.116	981	989	997	rBV6	4746	13416	0.96%	0.120%
18	7.208	997	1004	1011	rVV4	4581	10960	0.78%	0.098%
19	7.305	1011	1020	1039	rVB	293262	650985	46.51%	5.814%
20	7.488	1045	1050	1055	rVB4	819	1589	0.11%	0.014%
21	7.763	1092	1095	1103	rVB4	1047	1956	0.14%	0.017%
22	7.958	1119	1127	1136	rBV9	4885	13314	0.95%	0.119%
23	8.269	1173	1178	1181	rBV3	998	1595	0.11%	0.014%
24	8.324	1181	1187	1199	rBV	160410	266229	19.02%	2.378%
25	8.513	1211	1218	1220	rBV4	955	1731	0.12%	0.015%
26	8.647	1228	1240	1250	rBV	740165	1156334	82.61%	10.327%
27	8.842	1270	1272	1281	rVB6	1361	2083	0.15%	0.019%
28	8.951	1285	1290	1303	rVV	110577	174438	12.46%	1.558%
29	9.110	1311	1316	1322	rVB5	1300	1876	0.13%	0.017%
30	9.390	1356	1362	1363	rVV	137313	166316	11.88%	1.485%
31	9.415	1364	1366	1384	rVV	225850	396439	28.32%	3.540%
32	9.555	1387	1389	1395	rVV4	2817	5447	0.39%	0.049%
33	9.616	1395	1399	1403	rVV3	6456	10893	0.78%	0.097%
34	9.653	1403	1405	1415	rVV5	1792	3829	0.27%	0.034%
35	9.756	1419	1422	1425	rVV6	1210	1624	0.12%	0.015%
36	9.817	1428	1432	1438	rBV5	1647	3153	0.23%	0.028%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
 Title : VOC Analysis

37	10.055	1465	1471	1486	rBV	788616	1116414	79.76%	9.970%
38	10.268	1501	1506	1508	rBV4	998	1552	0.11%	0.014%
39	10.299	1508	1511	1518	rVB6	2428	4744	0.34%	0.042%
40	10.360	1518	1521	1525	rBV5	2222	2963	0.21%	0.026%
41	10.585	1552	1558	1564	rBV4	1571	2463	0.18%	0.022%
42	10.646	1564	1568	1573	rBV3	1301	1988	0.14%	0.018%
43	10.780	1582	1590	1594	rBV6	4015	7572	0.54%	0.068%
44	10.860	1597	1603	1606	rBV5	1992	3059	0.22%	0.027%
45	10.890	1606	1608	1613	rVB3	2839	3838	0.27%	0.034%
46	10.945	1613	1617	1623	rBV5	2512	4481	0.32%	0.040%
47	11.085	1633	1640	1642	rBV5	3426	5520	0.39%	0.049%
48	11.201	1651	1659	1672	rBV	439886	649325	46.39%	5.799%
49	11.317	1675	1678	1680	rBV4	1278	1716	0.12%	0.015%
50	11.384	1687	1689	1694	rVB5	3144	4789	0.34%	0.043%
51	11.433	1694	1697	1700	rBV4	2598	3997	0.29%	0.036%
52	11.475	1701	1704	1710	rVB	9890	13596	0.97%	0.121%
53	11.628	1724	1729	1734	rVB6	2400	4491	0.32%	0.040%
54	11.677	1734	1737	1740	rBV3	2174	2863	0.20%	0.026%
55	11.713	1740	1743	1746	rVV3	6357	6638	0.47%	0.059%
56	11.756	1746	1750	1754	rVV4	3187	4646	0.33%	0.041%
57	11.841	1758	1764	1769	rBV7	1439	3126	0.22%	0.028%
58	11.890	1769	1772	1776	rBV5	2202	3092	0.22%	0.028%
59	12.024	1789	1794	1803	rBV	869337	1111019	79.37%	9.922%
60	12.164	1813	1817	1821	rVB4	2051	3385	0.24%	0.030%
61	12.250	1827	1831	1835	rBV5	1748	3569	0.25%	0.032%
62	12.323	1837	1843	1854	rVV	844015	1067845	76.29%	9.536%
63	12.420	1856	1859	1864	rVV	11080	15360	1.10%	0.137%
64	12.469	1864	1867	1873	rVB6	3221	4340	0.31%	0.039%
65	12.536	1875	1878	1880	rBV4	1977	2517	0.18%	0.022%
66	12.762	1912	1915	1919	rVB5	3347	3934	0.28%	0.035%
67	12.823	1922	1925	1927	rBV4	1357	2167	0.15%	0.019%
68	12.969	1945	1949	1955	rVB8	5866	10159	0.73%	0.091%
69	13.042	1958	1961	1965	rVB5	2001	2288	0.16%	0.020%
70	13.152	1975	1979	1983	rBV5	1765	3001	0.21%	0.027%
71	13.268	1992	1998	2000	rBV2	9229	14319	1.02%	0.128%
72	13.384	2013	2017	2021	rBV3	4968	6897	0.49%	0.062%
73	13.506	2034	2037	2040	rBV5	1829	2062	0.15%	0.018%
74	13.579	2046	2049	2051	rBV4	2839	3479	0.25%	0.031%
75	13.780	2077	2082	2088	rVB	39429	57387	4.10%	0.512%
76	13.847	2088	2093	2097	rVB6	3502	5884	0.42%	0.053%

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 Title : VOC Analysis

77	14.036	2120	2124	2128	rBV2	8455	10615	0.76%	0.095%
78	14.103	2132	2135	2138	rVV3	3545	5333	0.38%	0.048%
79	14.140	2138	2141	2144	rVB4	2730	3267	0.23%	0.029%
80	14.365	2174	2178	2183	rBV8	2079	3328	0.24%	0.030%
81	14.639	2216	2223	2227	rBV	26276	35041	2.50%	0.313%
82	14.755	2239	2242	2243	rBV3	6225	6540	0.47%	0.058%
83	14.780	2243	2246	2254	rVB	22820	31852	2.28%	0.284%
84	14.926	2268	2270	2277	rVB6	2001	3299	0.24%	0.029%
85	15.127	2301	2303	2307	rBV5	1745	1947	0.14%	0.017%
86	15.206	2313	2316	2324	rVB2	8019	11824	0.84%	0.106%
87	15.377	2340	2344	2347	rBV3	5986	8553	0.61%	0.076%
88	15.487	2356	2362	2370	rBV4	10857	22761	1.63%	0.203%
89	15.615	2378	2383	2386	rBV4	15766	26034	1.86%	0.232%
90	15.651	2386	2389	2396	rVB4	9794	15996	1.14%	0.143%
91	15.816	2412	2416	2417	rBV4	3107	3756	0.27%	0.034%
92	15.834	2417	2419	2429	rVB5	5843	11933	0.85%	0.107%
93	15.993	2440	2445	2448	rVB7	3460	6033	0.43%	0.054%
94	16.084	2455	2460	2466	rBV6	3968	7643	0.55%	0.068%
95	16.200	2477	2479	2483	rVB4	2468	2266	0.16%	0.020%
96	16.328	2492	2500	2510	rVB	48776	97235	6.95%	0.868%
97	16.475	2519	2524	2527	rVB4	1084	2176	0.16%	0.019%
98	16.535	2529	2534	2539	rVV7	3327	7109	0.51%	0.063%
99	16.603	2542	2545	2549	rVB4	3471	5012	0.36%	0.045%
100	16.688	2550	2559	2566	rVB3	12543	28778	2.06%	0.257%

Sum of corrected areas: 11197505

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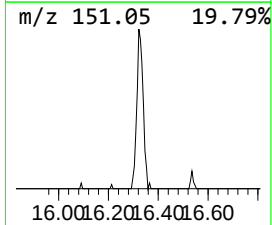
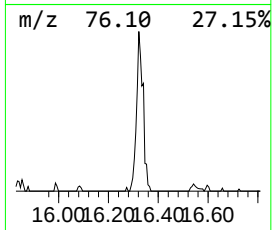
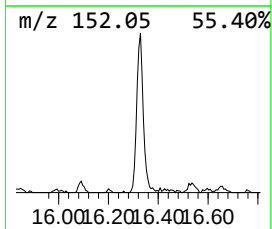
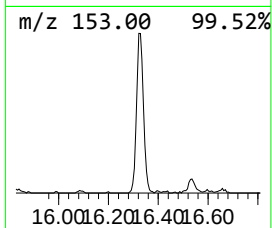
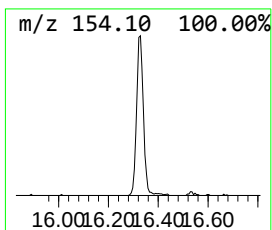
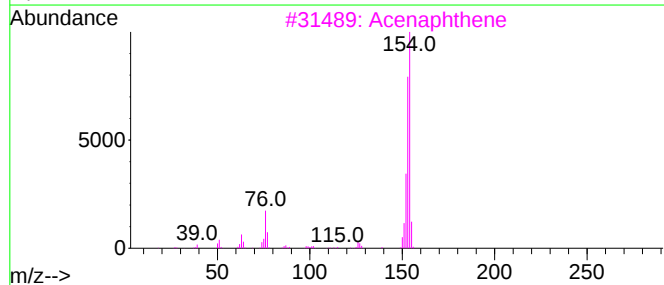
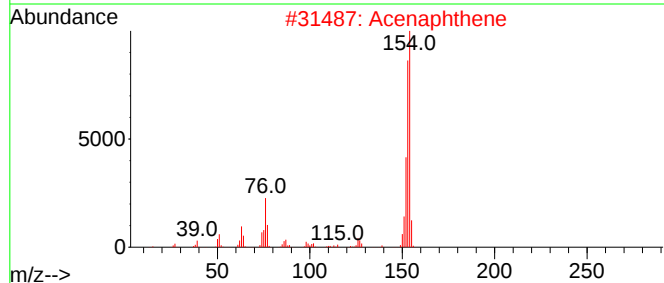
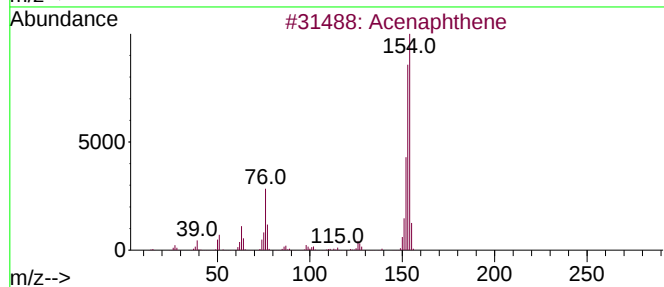
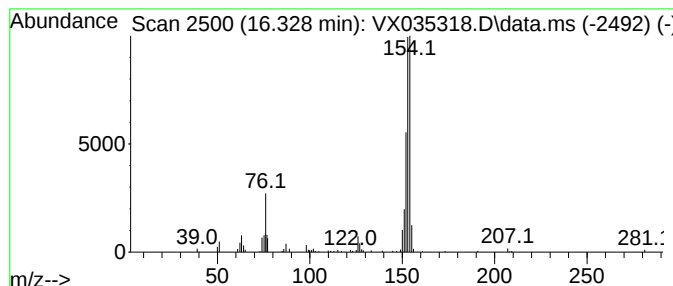
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Hexa-2,4-diyn-1-ylbenzene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.328	4.38 ug/L	97235	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acenaphthene	154	C12H10	000083-32-9	90
2			Acenaphthene	154	C12H10	000083-32-9	81
3			Acenaphthene	154	C12H10	000083-32-9	76
4			Acenaphthene	154	C12H10	000083-32-9	70
5			Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexa-2,4-diyn-1...	16.328	4.4	ug/L	97235	3	12.024	1111020	50.0