

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042623\
 Data File : VX035306.D
 Acq On : 26 Apr 2023 12:31
 Operator : JC/MD
 Sample : 02479-05ME
 Misc : 4.18g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EW946ME

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: VX035306.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	26	28	32	rVB3	1790	1767	0.15%	0.018%
2	1.367	42	46	67	rVB	59291	123276	10.16%	1.235%
3	1.672	92	96	99	rBV	27567	41151	3.39%	0.412%
4	2.288	191	197	213	rBV	234692	374342	30.86%	3.751%
5	2.605	248	249	251	rBV	223	178	0.01%	0.002%
6	2.666	257	259	264	rVB2	385	403	0.03%	0.004%
7	2.721	264	268	273	rBV4	808	1304	0.11%	0.013%
8	2.788	273	279	284	rBV4	3842	7218	0.60%	0.072%
9	3.032	317	319	321	rBV3	229	260	0.02%	0.003%
10	3.184	341	344	347	rBV2	261	356	0.03%	0.004%
11	3.215	347	349	352	rBV2	217	261	0.02%	0.003%
12	3.300	360	363	366	rBV2	280	318	0.03%	0.003%
13	3.434	379	385	388	rBV4	1122	2154	0.18%	0.022%
14	3.550	400	404	405	rBV	311	321	0.03%	0.003%
15	3.733	432	434	436	rVB2	209	173	0.01%	0.002%
16	4.300	522	527	532	rVB2	385	786	0.06%	0.008%
17	4.477	548	556	586	rBV	63414	238091	19.63%	2.386%
18	4.885	622	623	625	rBV	328	265	0.02%	0.003%
19	5.050	639	650	670	rBV2	145353	465813	38.40%	4.667%
20	5.556	725	733	740	rVB2	1571	3964	0.33%	0.040%
21	5.611	740	742	743	rBV	321	186	0.02%	0.002%
22	5.659	747	750	756	rVB2	226	365	0.03%	0.004%
23	5.806	772	774	776	rBV	235	215	0.02%	0.002%
24	5.964	787	800	819	rBV2	422562	1213064	100.00%	12.155%
25	6.361	856	865	872	rBV6	2441	6653	0.55%	0.067%
26	6.458	879	881	885	rVB3	235	207	0.02%	0.002%
27	6.531	891	893	895	rBV2	358	376	0.03%	0.004%
28	6.665	913	915	918	rBV2	187	214	0.02%	0.002%
29	6.757	920	930	946	rBV	419872	1013401	83.54%	10.154%
30	7.013	967	972	978	rVB4	858	1755	0.14%	0.018%
31	7.123	983	990	997	rVB9	3655	10835	0.89%	0.109%
32	7.202	997	1003	1012	rBV4	3838	9525	0.79%	0.095%
33	7.305	1012	1020	1035	rVB	250097	545953	45.01%	5.470%
34	7.482	1044	1049	1053	rBV2	838	1441	0.12%	0.014%
35	7.580	1064	1065	1069	rBV	356	300	0.02%	0.003%
36	7.696	1083	1084	1086	rBV	240	188	0.02%	0.002%

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37	7.793	1096	1100	1101	rBV2	220	298	0.02%	0.003%
38	7.964	1120	1128	1135	rBV5	3238	8959	0.74%	0.090%
39	8.068	1144	1145	1151	rVB5	490	675	0.06%	0.007%
40	8.128	1151	1155	1158	rVB2	219	293	0.02%	0.003%
41	8.263	1174	1177	1180	rBV3	497	538	0.04%	0.005%
42	8.324	1181	1187	1199	rBV	134119	225038	18.55%	2.255%
43	8.427	1202	1204	1212	rVB5	1149	2018	0.17%	0.020%
44	8.488	1212	1214	1215	rBV	600	392	0.03%	0.004%
45	8.586	1228	1230	1232	rBV2	458	456	0.04%	0.005%
46	8.647	1234	1240	1255	rVV	636814	1008503	83.14%	10.105%
47	8.915	1279	1284	1285	rBV4	1167	1339	0.11%	0.013%
48	8.952	1285	1290	1307	rVB	96079	147012	12.12%	1.473%
49	9.195	1328	1330	1332	rVB	389	372	0.03%	0.004%
50	9.226	1332	1335	1336	rBV2	387	332	0.03%	0.003%
51	9.275	1339	1343	1351	rVB3	1560	2426	0.20%	0.024%
52	9.390	1356	1362	1363	rBV	105947	132356	10.91%	1.326%
53	9.616	1395	1399	1403	rVB2	2590	3285	0.27%	0.033%
54	9.720	1414	1416	1418	rBV2	361	319	0.03%	0.003%
55	9.756	1421	1422	1424	rVB	491	214	0.02%	0.002%
56	9.787	1425	1427	1429	rBV	259	201	0.02%	0.002%
57	9.823	1429	1433	1437	rBV5	1710	2994	0.25%	0.030%
58	9.909	1442	1447	1451	rVB3	2007	2669	0.22%	0.027%
59	10.006	1459	1463	1465	rBV4	1213	1612	0.13%	0.016%
60	10.055	1465	1471	1489	rVV	801292	1148977	94.72%	11.513%
61	10.183	1489	1492	1494	rVV2	697	997	0.08%	0.010%
62	10.232	1498	1500	1503	rVB3	343	211	0.02%	0.002%
63	10.311	1509	1513	1518	rVB4	1882	3723	0.31%	0.037%
64	10.360	1518	1521	1527	rVB4	3127	4358	0.36%	0.044%
65	10.445	1532	1535	1536	rBV2	444	510	0.04%	0.005%
66	10.585	1551	1558	1561	rBV4	1494	2726	0.22%	0.027%
67	10.652	1563	1569	1575	rBV	12752	21295	1.76%	0.213%
68	10.738	1581	1583	1584	rBV	299	222	0.02%	0.002%
69	10.780	1586	1590	1594	rVB3	2393	2729	0.22%	0.027%
70	10.817	1594	1596	1598	rBV2	359	320	0.03%	0.003%
71	10.945	1613	1617	1624	rVB	10263	14993	1.24%	0.150%
72	11.000	1624	1626	1628	rBV2	565	480	0.04%	0.005%
73	11.030	1628	1631	1634	rVB3	972	957	0.08%	0.010%
74	11.085	1634	1640	1642	rBV6	2927	5617	0.46%	0.056%
75	11.201	1650	1659	1673	rBV	360228	554182	45.68%	5.553%
76	11.311	1674	1677	1681	rBV3	1216	1781	0.15%	0.018%

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77	11.439	1693	1698	1699	rBV3	1819	2892	0.24%	0.029%
78	11.475	1702	1704	1710	rVB3	8955	12737	1.05%	0.128%
79	11.573	1718	1720	1721	rBV2	372	276	0.02%	0.003%
80	11.683	1735	1738	1740	rBV2	2655	3129	0.26%	0.031%
81	11.713	1740	1743	1746	rVV2	3258	3514	0.29%	0.035%
82	11.847	1758	1765	1766	rBV5	1378	2626	0.22%	0.026%
83	11.939	1777	1780	1782	rBV4	1109	1420	0.12%	0.014%
84	11.975	1783	1786	1788	rVB3	2415	2474	0.20%	0.025%
85	12.024	1789	1794	1804	rBV	913464	1164756	96.02%	11.671%
86	12.158	1813	1816	1825	rVB6	5264	8970	0.74%	0.090%
87	12.250	1826	1831	1833	rBV4	2635	4052	0.33%	0.041%
88	12.323	1837	1843	1856	rVV	730916	935081	77.08%	9.369%
89	12.420	1857	1859	1863	rVB4	4146	4539	0.37%	0.045%
90	13.268	1996	1998	1999	rBV2	3000	2836	0.23%	0.028%
91	13.524	2033	2040	2041	rBV5	3520	7167	0.59%	0.072%
92	13.774	2077	2081	2090	rBV	75085	106999	8.82%	1.072%
93	14.640	2219	2223	2233	rVB	31984	46566	3.84%	0.467%
94	14.780	2242	2246	2250	rVB	35895	44251	3.65%	0.443%
95	15.475	2356	2360	2370	rVB	20112	35616	2.94%	0.357%
96	15.615	2378	2383	2386	rBV	36301	57048	4.70%	0.572%
97	15.810	2411	2415	2416	rBV3	8336	10776	0.89%	0.108%
98	16.084	2457	2460	2467	rVB5	6396	10237	0.84%	0.103%
99	16.328	2493	2500	2509	rBV	58084	115043	9.48%	1.153%
100	16.657	2549	2554	2556	rBV3	13788	23700	1.95%	0.237%

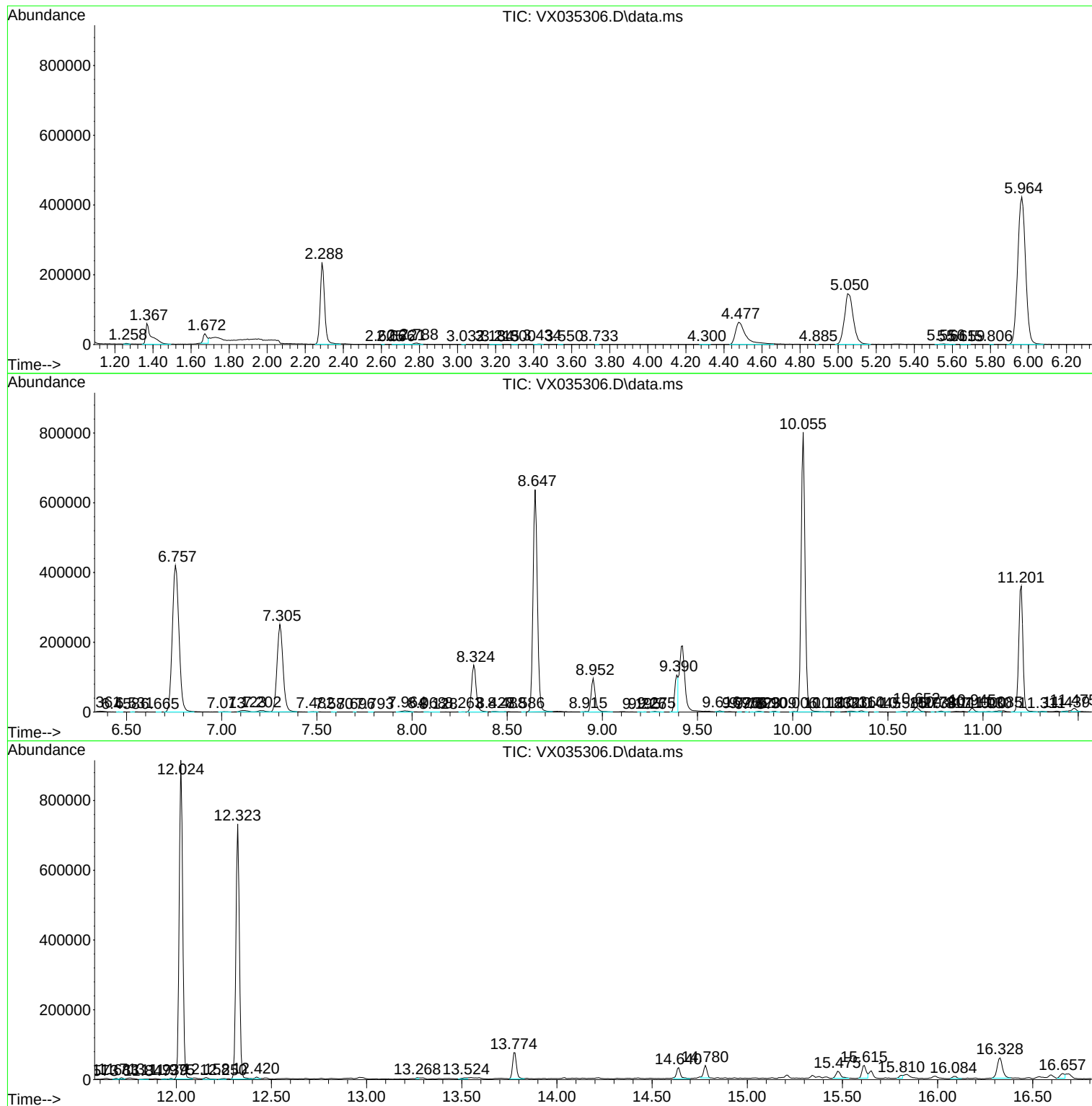
Sum of corrected areas: 9980163

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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



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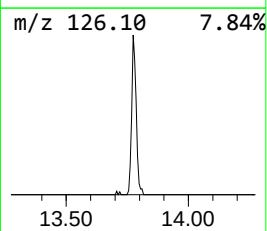
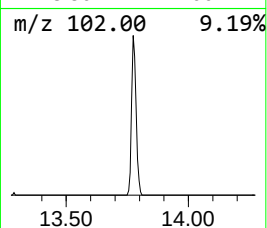
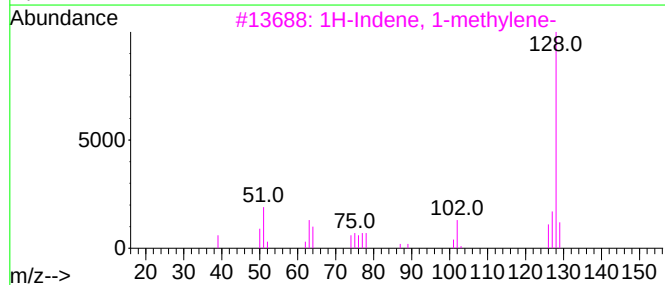
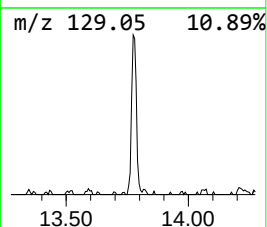
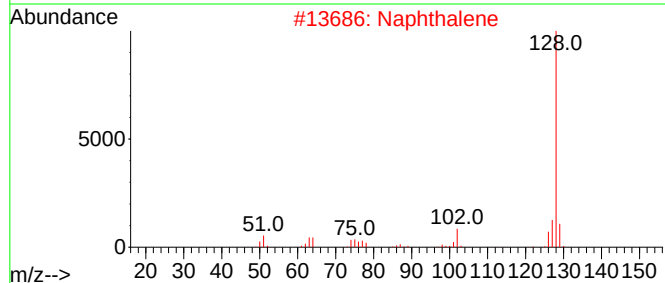
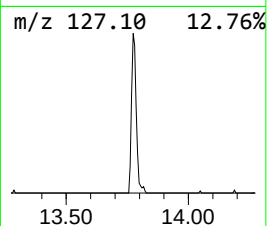
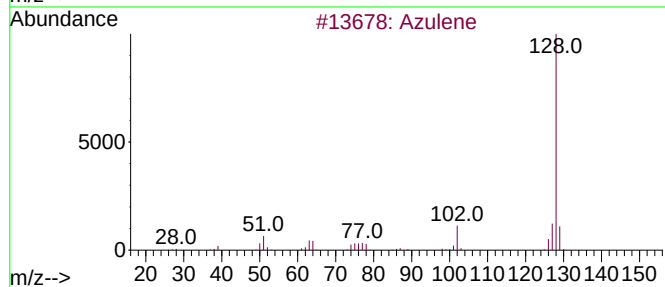
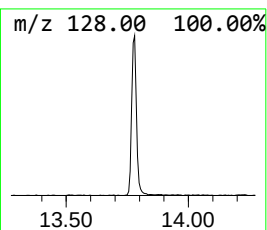
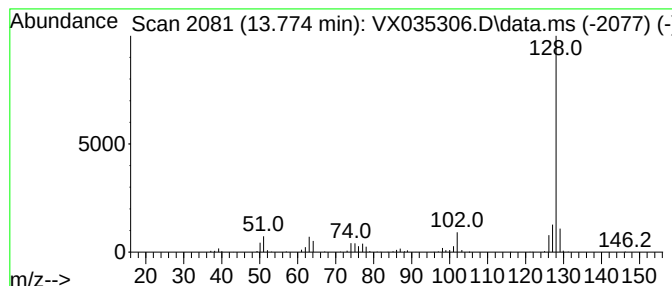
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM041823WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Azulene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	4.59 ug/L	106999	1,4-Dichlorobenzene-d4	12.024

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



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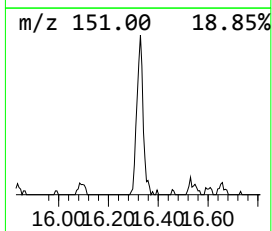
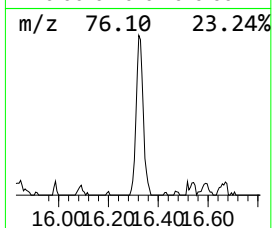
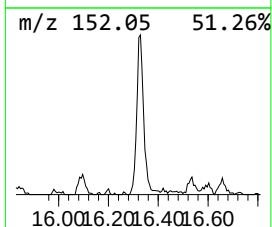
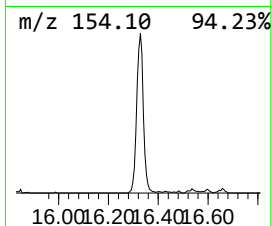
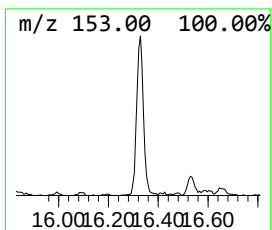
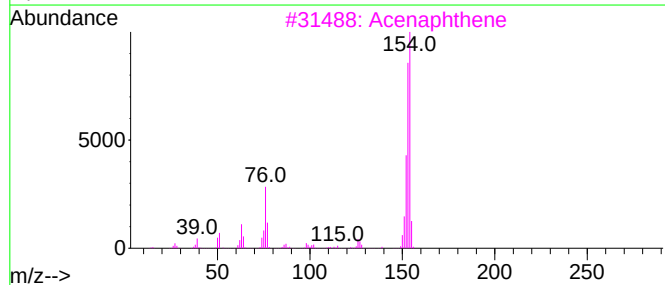
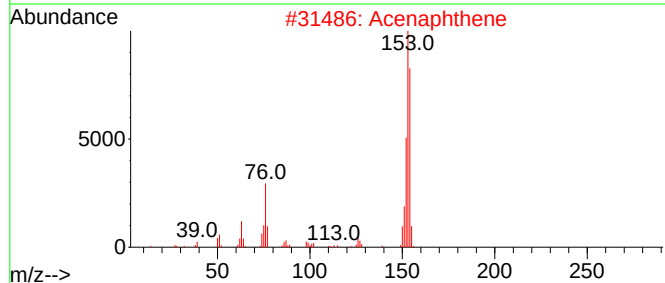
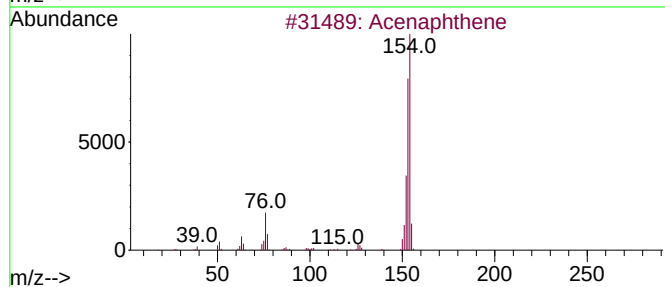
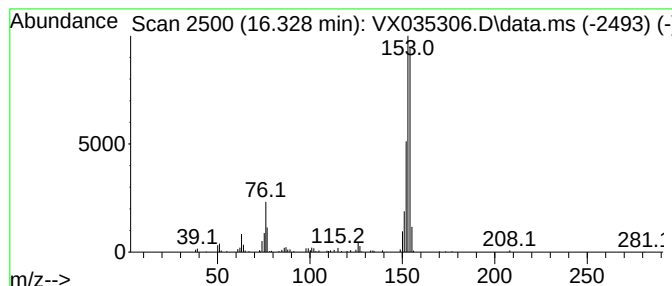
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM041823WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Naphthalene, 2-ethenyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.328	4.94 ug/L	115043	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acenaphthene	154	C12H10	000083-32-9	93
2			Acenaphthene	154	C12H10	000083-32-9	89
3			Acenaphthene	154	C12H10	000083-32-9	81
4			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	64
5			Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	59



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Azulene	13.774	4.6	ug/L	106999	3	12.024	1164760	50.0
Naphthalene, 2-...	16.328	4.9	ug/L	115043	3	12.024	1164760	50.0