

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081121\
 Data File : VX023655.D
 Acq On : 11 Aug 2021 17:40
 Operator : JC/MD
 Sample : M3364-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 DBK86

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\SFAMXML081121WMA.M

Title : VOC Analysis

Signal : TIC: VX023655.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	25	27	33	rBV4	3831	5489	0.50%	0.061%
2	1.368	43	46	54	rVB	121316	120716	11.06%	1.333%
3	1.666	90	95	103	rBV	97138	123196	11.28%	1.360%
4	2.306	194	200	209	rBV	220740	365855	33.51%	4.040%
5	2.386	210	213	221	rVB	4649	8525	0.78%	0.094%
6	2.660	255	258	260	rBV2	525	593	0.05%	0.007%
7	2.794	276	280	285	rBV3	1087	1713	0.16%	0.019%
8	2.953	298	306	307	rBV3	795	1331	0.12%	0.015%
9	3.123	327	334	342	rVV2	4992	11280	1.03%	0.125%
10	3.623	411	416	423	rVB4	1270	2678	0.25%	0.030%
11	4.465	544	554	571	rBV	92353	261393	23.94%	2.887%
12	4.794	605	608	610	rBV2	292	337	0.03%	0.004%
13	4.916	625	628	632	rVB2	313	528	0.05%	0.006%
14	5.068	640	653	669	rVV	141032	430049	39.39%	4.749%
15	5.227	675	679	683	rVB2	695	783	0.07%	0.009%
16	5.568	727	735	746	rVB6	1215	3460	0.32%	0.038%
17	5.977	790	802	820	rBV2	370937	1091757	100.00%	12.056%
18	6.336	856	861	863	rBV3	492	867	0.08%	0.010%
19	6.550	893	896	897	rBV3	335	424	0.04%	0.005%
20	6.769	922	932	946	rBV	328701	772952	70.80%	8.536%
21	7.019	968	973	976	rBV3	360	497	0.05%	0.005%
22	7.117	983	989	997	rVB5	5227	10928	1.00%	0.121%
23	7.318	1012	1022	1037	rBV	232651	501835	45.97%	5.542%
24	7.586	1060	1066	1067	rBV2	414	485	0.04%	0.005%
25	7.647	1074	1076	1079	rVB2	343	387	0.04%	0.004%
26	7.684	1079	1082	1087	rBV2	644	842	0.08%	0.009%
27	7.812	1101	1103	1107	rVB4	793	913	0.08%	0.010%
28	7.927	1117	1122	1129	rVB3	2183	4283	0.39%	0.047%
29	8.171	1161	1162	1165	rBV	313	342	0.03%	0.004%
30	8.330	1181	1188	1203	rVV	150738	237942	21.79%	2.628%
31	8.470	1206	1211	1219	rBV4	1931	3897	0.36%	0.043%
32	8.653	1234	1241	1248	rBV	588751	898744	82.32%	9.925%
33	8.720	1248	1252	1258	rVB2	14155	22999	2.11%	0.254%
34	8.952	1284	1290	1299	rBV	108112	157855	14.46%	1.743%
35	9.135	1318	1320	1324	rVB	464	513	0.05%	0.006%
36	9.281	1339	1344	1351	rVB4	2283	3504	0.32%	0.039%

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 Title : VOC Analysis

37	9.391	1355	1362	1380	rBV	395273	588773	53.93%	6.502%
38	9.866	1437	1440	1442	rVB2	343	362	0.03%	0.004%
39	9.890	1442	1444	1446	rBV2	388	347	0.03%	0.004%
40	9.945	1451	1453	1460	rVV2	299	375	0.03%	0.004%
41	10.055	1465	1471	1487	rVV	677813	928592	85.05%	10.254%
42	10.201	1490	1495	1499	rVB3	1645	2438	0.22%	0.027%
43	10.244	1499	1502	1506	rBV3	291	442	0.04%	0.005%
44	10.305	1508	1512	1519	rVB3	2259	3394	0.31%	0.037%
45	10.592	1554	1559	1561	rVB2	341	352	0.03%	0.004%
46	10.646	1565	1568	1575	rVB5	1091	1953	0.18%	0.022%
47	10.756	1585	1586	1589	rVB	484	351	0.03%	0.004%
48	10.860	1598	1603	1606	rVB3	927	1528	0.14%	0.017%
49	10.963	1617	1620	1626	rVB3	1925	2649	0.24%	0.029%
50	11.079	1635	1639	1642	rBV2	342	470	0.04%	0.005%
51	11.122	1642	1646	1652	rBV2	4050	4852	0.44%	0.054%
52	11.195	1652	1658	1666	rBV	415026	519607	47.59%	5.738%
53	11.311	1674	1677	1683	rVB4	2971	4538	0.42%	0.050%
54	11.469	1697	1703	1704	rBV4	1027	1597	0.15%	0.018%
55	11.543	1712	1715	1719	rBV2	633	915	0.08%	0.010%
56	11.616	1724	1727	1733	rVV2	1948	2520	0.23%	0.028%
57	11.683	1736	1738	1741	rVB3	578	545	0.05%	0.006%
58	11.713	1741	1743	1745	rBV	661	632	0.06%	0.007%
59	11.750	1745	1749	1754	rVB2	4559	6559	0.60%	0.072%
60	11.841	1762	1764	1770	rBV4	633	863	0.08%	0.010%
61	11.890	1770	1772	1775	rBV2	499	369	0.03%	0.004%
62	11.933	1775	1779	1783	rBV	2252	2922	0.27%	0.032%
63	12.024	1788	1794	1801	rBV	666062	810869	74.27%	8.954%
64	12.134	1807	1812	1813	rBV3	1303	2023	0.19%	0.022%
65	12.152	1813	1815	1819	rVB2	3288	3652	0.33%	0.040%
66	12.244	1825	1830	1835	rVB	32081	39596	3.63%	0.437%
67	12.323	1835	1843	1851	rVV	580713	728137	66.69%	8.041%
68	12.378	1851	1852	1857	rVV3	772	830	0.08%	0.009%
69	12.433	1857	1861	1866	rVB3	1052	1642	0.15%	0.018%
70	12.481	1866	1869	1873	rBV3	821	1122	0.10%	0.012%
71	12.622	1888	1892	1893	rVV2	1132	1292	0.12%	0.014%
72	12.646	1893	1896	1901	rVV3	3096	4385	0.40%	0.048%
73	12.701	1901	1905	1909	rVB	8594	9590	0.88%	0.106%
74	12.799	1918	1921	1923	rBV2	297	409	0.04%	0.005%
75	12.853	1927	1930	1933	rBV2	786	868	0.08%	0.010%
76	12.896	1933	1937	1938	rVB3	595	628	0.06%	0.007%

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 Title : VOC Analysis

77	12.927	1938	1942	1944	rVB2	666	793	0.07%	0.009%
78	12.975	1947	1950	1952	rBV4	682	914	0.08%	0.010%
79	13.030	1957	1959	1961	rVV	455	438	0.04%	0.005%
80	13.055	1961	1963	1968	rVB4	999	1272	0.12%	0.014%
81	13.170	1977	1982	1987	rVB	7599	8740	0.80%	0.097%
82	13.292	1998	2002	2007	rVV	17203	21329	1.95%	0.236%
83	13.341	2008	2010	2015	rVB2	709	860	0.08%	0.009%
84	13.420	2021	2023	2028	rBV4	881	1235	0.11%	0.014%
85	13.548	2040	2044	2046	rBV2	549	785	0.07%	0.009%
86	13.591	2049	2051	2054	rVB3	734	612	0.06%	0.007%
87	13.780	2077	2082	2087	rBV	2581	2891	0.26%	0.032%
88	13.841	2089	2092	2094	rBV2	296	453	0.04%	0.005%
89	13.865	2094	2096	2100	rVB3	413	509	0.05%	0.006%
90	13.926	2102	2106	2110	rBV2	310	469	0.04%	0.005%
91	13.963	2110	2112	2115	rBV2	358	465	0.04%	0.005%
92	14.134	2135	2140	2144	rBV3	655	1199	0.11%	0.013%
93	14.597	2212	2216	2219	rVV	8442	10387	0.95%	0.115%
94	14.640	2219	2223	2232	rVB	44376	54169	4.96%	0.598%
95	14.725	2234	2237	2241	rVB3	1825	2298	0.21%	0.025%
96	14.780	2241	2246	2257	rBV	123597	159686	14.63%	1.763%
97	15.560	2371	2374	2375	rBV2	478	608	0.06%	0.007%
98	15.615	2379	2383	2389	rVV3	4687	7197	0.66%	0.079%
99	15.822	2413	2417	2418	rBV3	813	1171	0.11%	0.013%
100	16.328	2494	2500	2508	rVB2	24874	44311	4.06%	0.489%

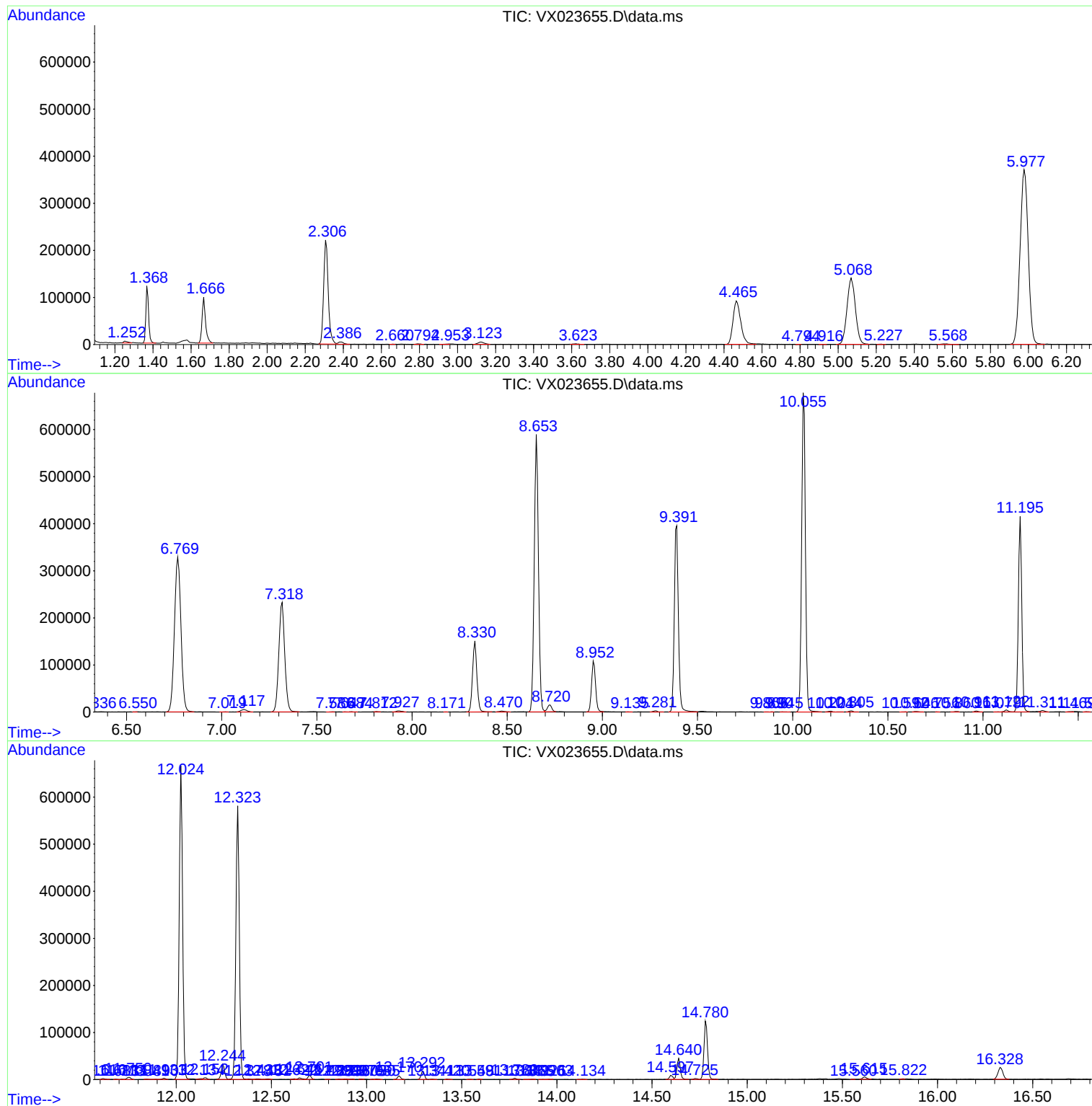
Sum of corrected areas: 9055671

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML081121WMA.M
Quant Title : VOC Analysis

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



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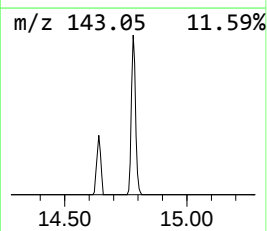
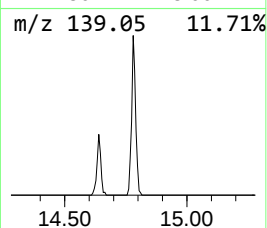
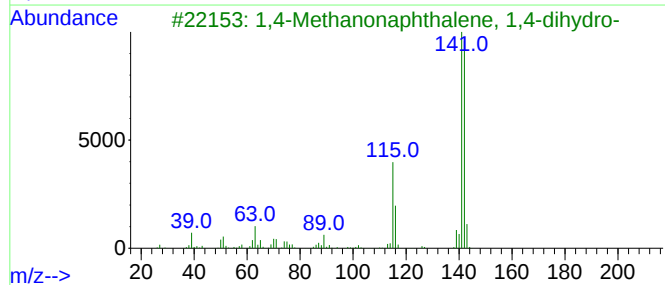
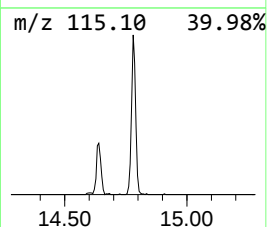
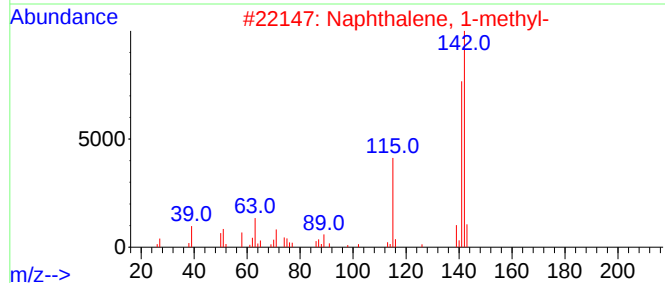
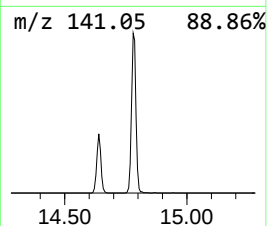
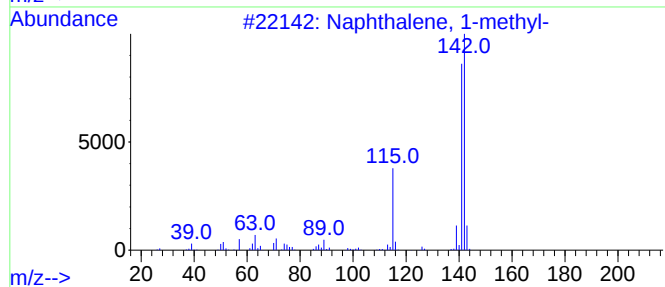
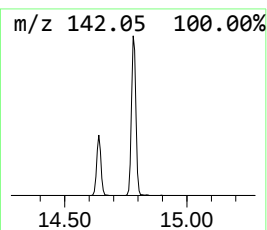
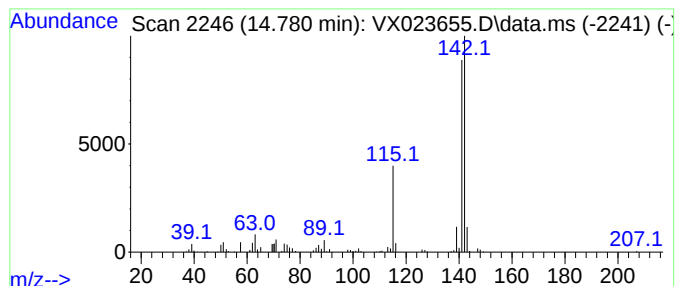
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML081121WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 1,4-Methanonaphthalene, 1,4... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	9.85 ug/L	159686	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94
4			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	94
5			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	94



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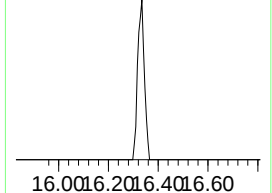
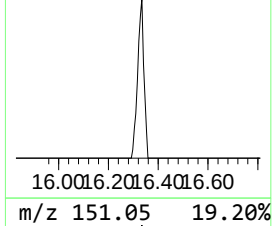
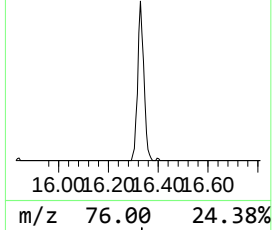
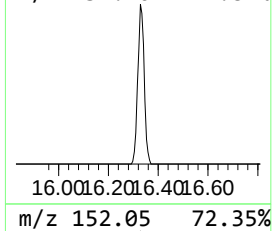
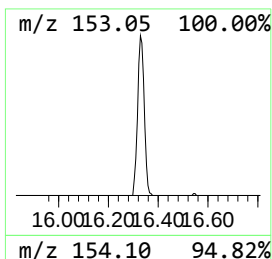
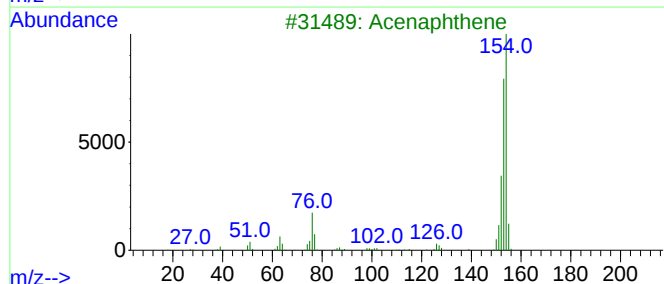
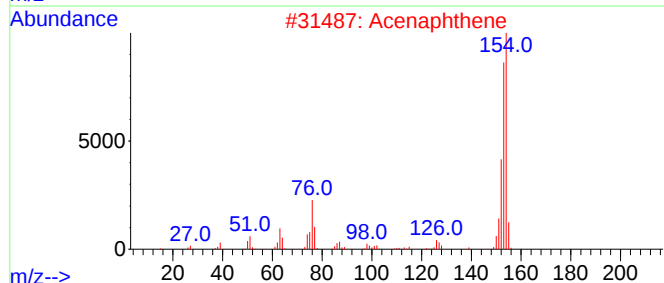
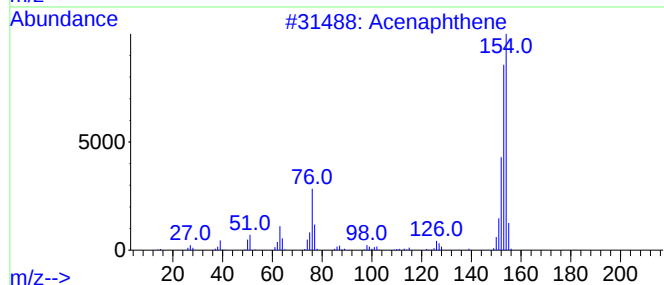
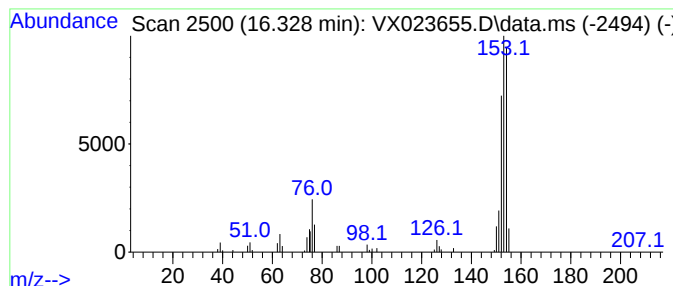
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML081121WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.328	2.73 ug/L	44311	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acenaphthene			154	C12H10	000083-32-9	76
2	Acenaphthene			154	C12H10	000083-32-9	70
3	Acenaphthene			154	C12H10	000083-32-9	68
4	Acenaphthene			154	C12H10	000083-32-9	64
5	Hexa-2,4-diyn-1-ylbenzene			154	C12H10	000520-74-1	58



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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
1,4-Methanonaph...	14.780	9.8	ug/L	159686	3	12.024	810869	50.0
Hexa-2,4-diyne-1...	16.328	2.7	ug/L	44311	3	12.024	810869	50.0