

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013125\
 Data File : VX044796.D
 Acq On : 31 Jan 2025 15:03
 Operator : JC/MD
 Sample : Q1189-02ME
 Misc : 16.96g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A44Q5ME

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\SFAMXML012825WMA.M

Title : VOC Analysis

Signal : TIC: VX044796.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	22	25	33	rBV2	14150	23954	2.37%	0.308%
2	1.368	43	46	51	rBV	82911	105214	10.41%	1.354%
3	1.563	72	78	79	rBV3	3934	6704	0.66%	0.086%
4	1.648	88	92	97	rBV	20306	30005	2.97%	0.386%
5	2.288	189	197	211	rBV	210856	346896	34.31%	4.466%
6	2.587	242	246	250	rBV2	850	1813	0.18%	0.023%
7	2.715	262	267	273	rVB	3002	5333	0.53%	0.069%
8	2.825	283	285	288	rVB2	612	654	0.06%	0.008%
9	2.940	298	304	316	rVV3	3939	10243	1.01%	0.132%
10	3.422	378	383	391	rBV4	1138	2698	0.27%	0.035%
11	4.477	547	556	580	rBV	48052	183574	18.15%	2.363%
12	5.050	639	650	666	rBV2	130827	390737	38.64%	5.030%
13	5.379	699	704	705	rBV3	1268	1886	0.19%	0.024%
14	5.446	714	715	720	rVB3	635	841	0.08%	0.011%
15	5.489	720	722	725	rVB3	581	674	0.07%	0.009%
16	5.544	727	731	734	rBV2	627	941	0.09%	0.012%
17	5.964	788	800	817	rBV3	348536	1011163	100.00%	13.017%
18	6.446	875	879	883	rVB2	426	636	0.06%	0.008%
19	6.757	918	930	950	rBV	240198	608407	60.17%	7.832%
20	7.110	984	988	989	rBV3	688	988	0.10%	0.013%
21	7.220	1002	1006	1009	rBV2	573	585	0.06%	0.008%
22	7.305	1011	1020	1038	rBV	204736	459265	45.42%	5.912%
23	7.866	1109	1112	1115	rBV2	465	733	0.07%	0.009%
24	8.269	1173	1178	1181	rVB2	537	877	0.09%	0.011%
25	8.324	1181	1187	1199	rBV	142360	246713	24.40%	3.176%
26	8.647	1233	1240	1258	rBV	484257	823068	81.40%	10.595%
27	8.909	1278	1283	1285	rBV3	1794	2524	0.25%	0.032%
28	8.952	1285	1290	1304	rVV	97541	156660	15.49%	2.017%
29	9.116	1316	1317	1323	rVB2	537	688	0.07%	0.009%
30	9.390	1355	1362	1377	rBV	198185	359129	35.52%	4.623%
31	9.610	1394	1398	1402	rVB6	1123	1713	0.17%	0.022%
32	9.708	1411	1414	1418	rVB3	901	1255	0.12%	0.016%
33	9.896	1442	1445	1451	rBV4	695	1069	0.11%	0.014%
34	10.006	1458	1463	1465	rBV3	588	811	0.08%	0.010%
35	10.055	1465	1471	1490	rVV	482571	730307	72.22%	9.401%
36	10.195	1492	1494	1498	rBV3	641	758	0.07%	0.010%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012825WMA.M
 Title : VOC Analysis

37	10.305	1509	1512	1516	rVB4	1367	2176	0.22%	0.028%
38	10.360	1516	1521	1525	rBV2	3816	4479	0.44%	0.058%
39	10.598	1556	1560	1564	rVV3	706	1305	0.13%	0.017%
40	10.646	1565	1568	1573	rVV5	1098	1672	0.17%	0.022%
41	10.780	1585	1590	1593	rVB3	878	1239	0.12%	0.016%
42	10.854	1596	1602	1604	rBV4	680	1305	0.13%	0.017%
43	10.951	1614	1618	1619	rBV2	573	831	0.08%	0.011%
44	11.189	1652	1657	1669	rBV	337990	462574	45.75%	5.955%
45	11.299	1672	1675	1679	rBV4	443	702	0.07%	0.009%
46	11.384	1686	1689	1693	rBV4	1458	1925	0.19%	0.025%
47	11.475	1700	1704	1708	rVB4	4795	6611	0.65%	0.085%
48	11.628	1724	1729	1730	rBV2	643	965	0.10%	0.012%
49	11.683	1734	1738	1739	rBV2	495	601	0.06%	0.008%
50	11.713	1740	1743	1747	rVB4	1948	2155	0.21%	0.028%
51	11.756	1747	1750	1754	rBV4	1675	2193	0.22%	0.028%
52	11.884	1769	1771	1774	rBV3	869	1221	0.12%	0.016%
53	11.939	1777	1780	1783	rBV3	1302	1794	0.18%	0.023%
54	11.975	1783	1786	1788	rVB3	760	992	0.10%	0.013%
55	12.018	1788	1793	1804	rBV	551449	721338	71.34%	9.286%
56	12.201	1822	1823	1826	rBV2	684	674	0.07%	0.009%
57	12.250	1826	1831	1833	rBV3	1876	2847	0.28%	0.037%
58	12.317	1837	1842	1850	rBV	582737	713694	70.58%	9.187%
59	12.420	1856	1859	1863	rVB3	5589	6381	0.63%	0.082%
60	12.561	1874	1882	1883	rBV5	1556	3264	0.32%	0.042%
61	12.616	1889	1891	1893	rBV2	689	584	0.06%	0.008%
62	12.689	1898	1903	1905	rBV4	996	1689	0.17%	0.022%
63	12.762	1911	1915	1920	rVB5	2292	3404	0.34%	0.044%
64	12.884	1931	1935	1942	rVV5	1918	4075	0.40%	0.052%
65	12.963	1945	1948	1954	rVB5	1439	2917	0.29%	0.038%
66	13.036	1956	1960	1965	rVB5	1177	1469	0.15%	0.019%
67	13.164	1976	1981	1985	rBV7	925	1826	0.18%	0.024%
68	13.219	1985	1990	1991	rBV2	968	1382	0.14%	0.018%
69	13.268	1994	1998	2000	rBV3	4325	5459	0.54%	0.070%
70	13.292	2000	2002	2008	rVB5	2756	3835	0.38%	0.049%
71	13.384	2012	2017	2018	rBV4	2161	2320	0.23%	0.030%
72	13.402	2018	2020	2025	rVB5	2076	2945	0.29%	0.038%
73	13.579	2046	2049	2051	rBV3	1291	1389	0.14%	0.018%
74	13.676	2062	2065	2067	rBV3	1060	1215	0.12%	0.016%
75	13.780	2077	2082	2089	rBV	9673	13859	1.37%	0.178%
76	13.841	2089	2092	2096	rBV3	2114	2036	0.20%	0.026%

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 ClientSampleId :
 A44Q5ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012825WMA.M
 Title : VOC Analysis

77	13.908	2100	2103	2104	rBV2	724	679	0.07%	0.009%
78	13.969	2112	2113	2115	rBV2	629	622	0.06%	0.008%
79	14.042	2121	2125	2127	rVB3	2945	3702	0.37%	0.048%
80	14.079	2127	2131	2132	rBV4	1089	1688	0.17%	0.022%
81	14.127	2136	2139	2142	rVV3	2373	2389	0.24%	0.031%
82	14.219	2150	2154	2157	rBV4	2410	3544	0.35%	0.046%
83	14.329	2167	2172	2175	rBV5	1838	3094	0.31%	0.040%
84	14.371	2177	2179	2182	rVB3	2183	2102	0.21%	0.027%
85	14.414	2184	2186	2188	rBV3	1212	1273	0.13%	0.016%
86	14.481	2195	2197	2200	rBV4	1425	2038	0.20%	0.026%
87	14.572	2210	2212	2216	rBV4	1130	1222	0.12%	0.016%
88	14.640	2216	2223	2226	rBV	9869	15271	1.51%	0.197%
89	14.755	2239	2242	2243	rBV3	3191	2911	0.29%	0.037%
90	14.780	2243	2246	2254	rVB	16149	22040	2.18%	0.284%
91	15.182	2309	2312	2313	rBV3	1844	1796	0.18%	0.023%
92	15.383	2342	2345	2346	rBV3	2803	3491	0.35%	0.045%
93	15.481	2355	2361	2373	rVB	19095	37577	3.72%	0.484%
94	15.615	2378	2383	2386	rVV	28907	46334	4.58%	0.596%
95	15.652	2386	2389	2398	rVB2	16808	26179	2.59%	0.337%
96	15.810	2411	2415	2417	rBV3	6581	10373	1.03%	0.134%
97	16.084	2457	2460	2467	rVB6	4631	7630	0.75%	0.098%
98	16.322	2496	2499	2508	rVB4	8288	20488	2.03%	0.264%
99	16.468	2520	2523	2528	rBV5	2943	4840	0.48%	0.062%
100	16.657	2549	2554	2569	rVB5	11573	34144	3.38%	0.440%

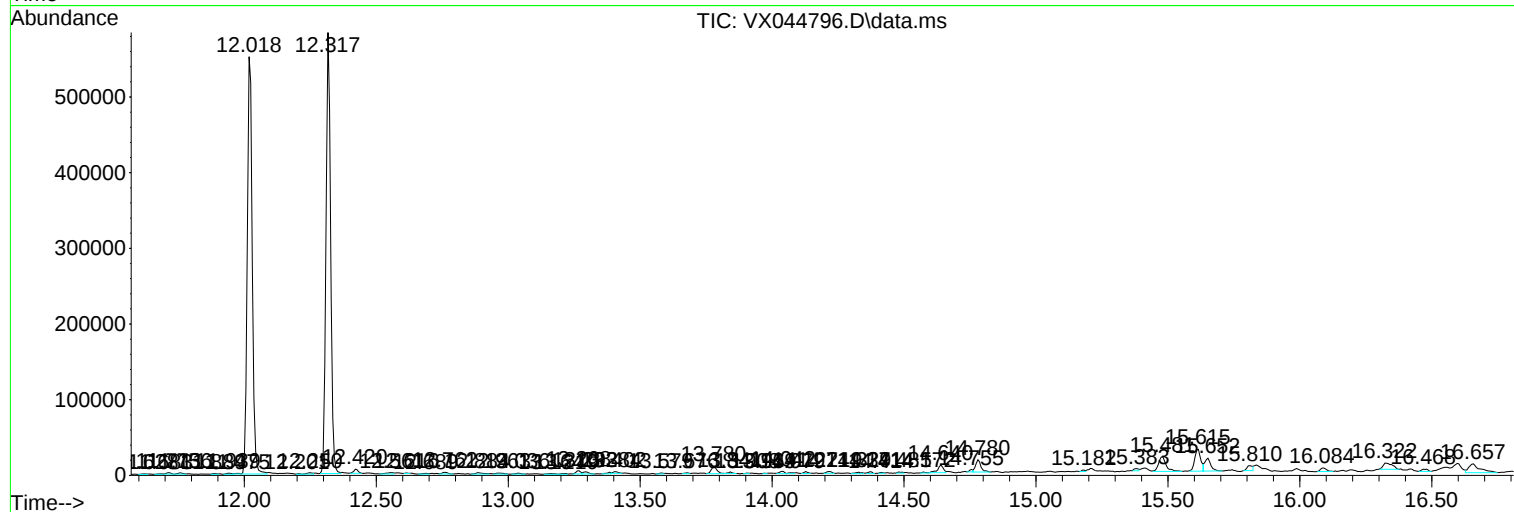
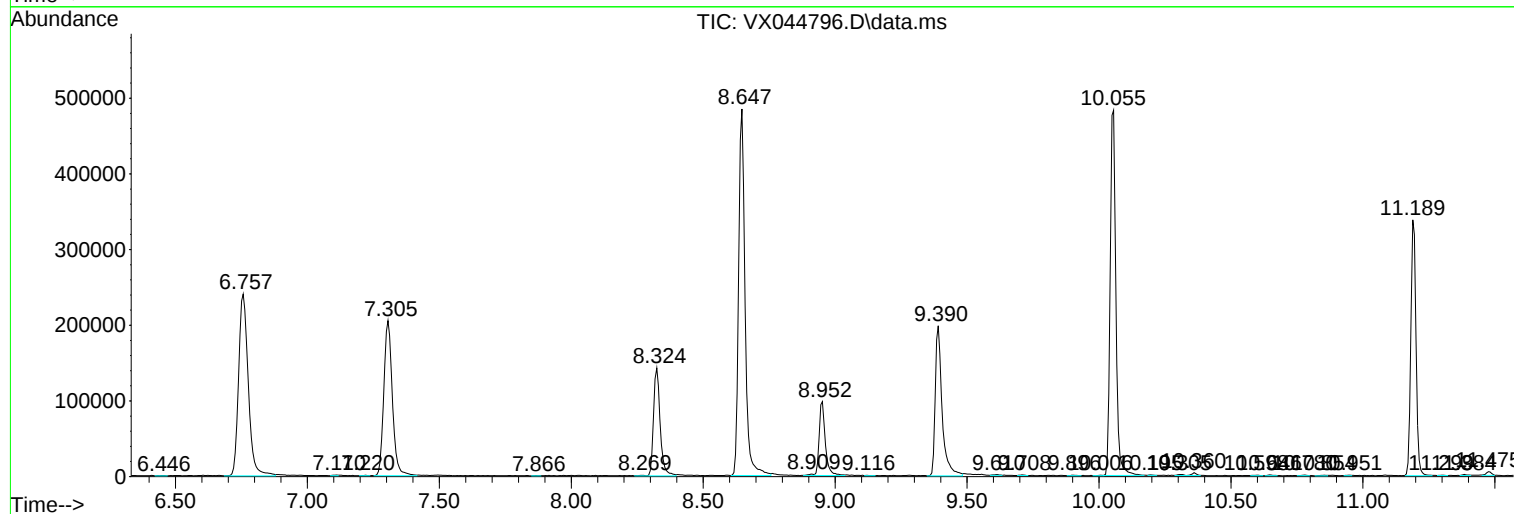
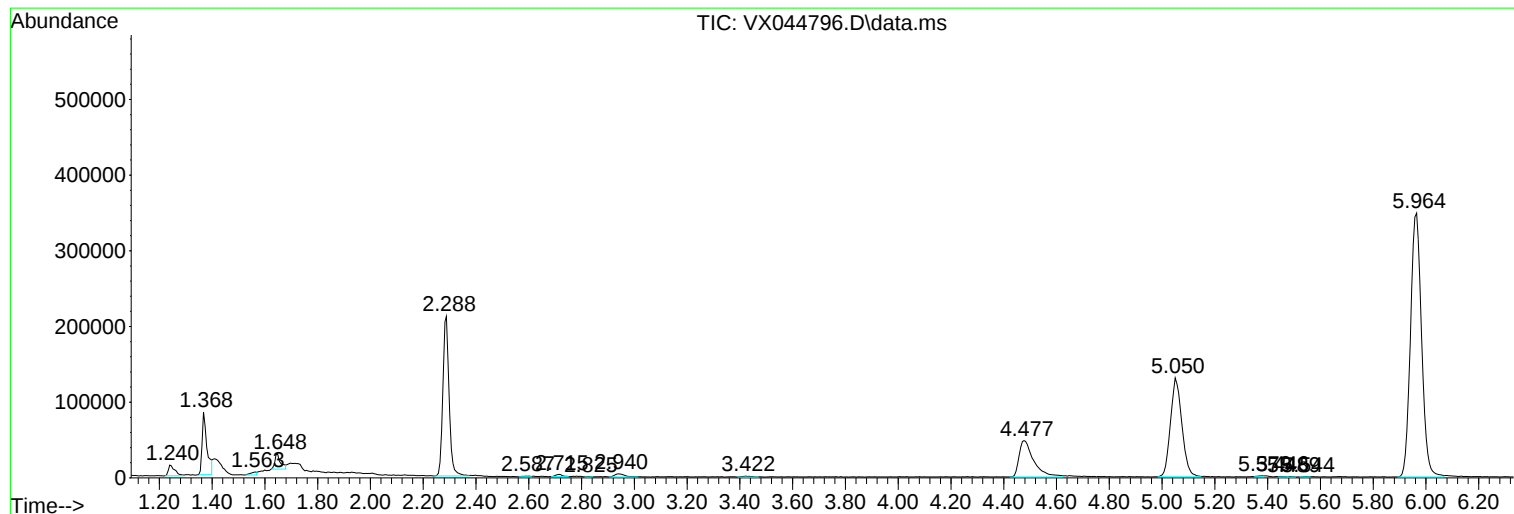
Sum of corrected areas: 7768285

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ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44Q5ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012825WMA.M
Quant Title : VOC Analysis

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



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Instrument :
MSVOA_X
ClientSampleId :
A44Q5ME

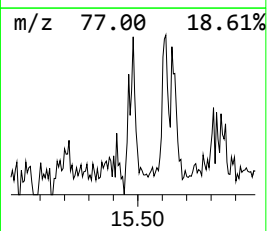
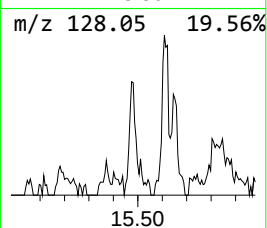
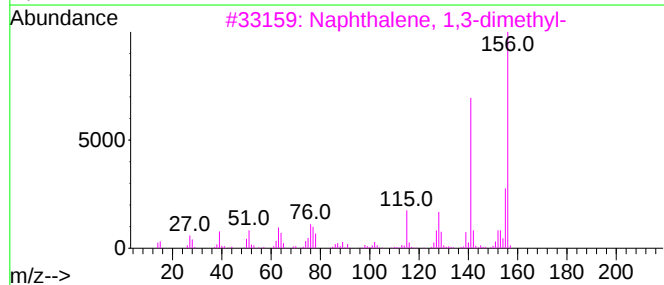
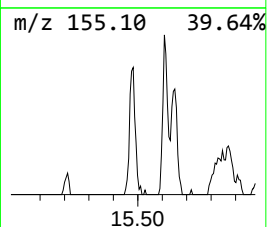
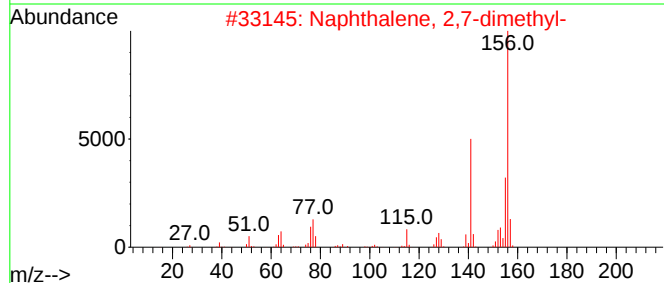
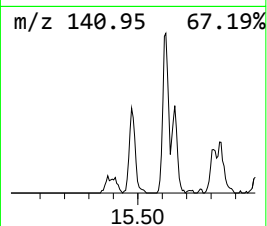
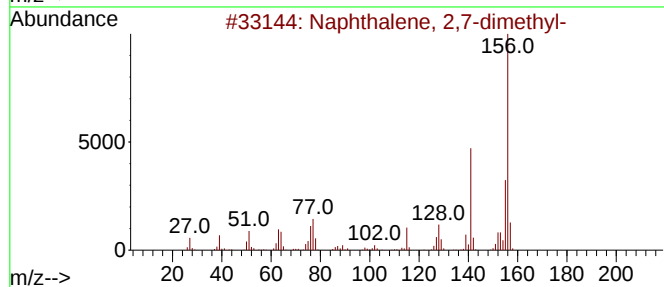
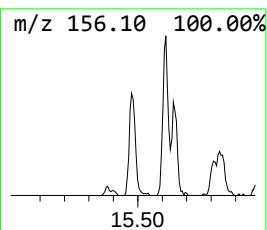
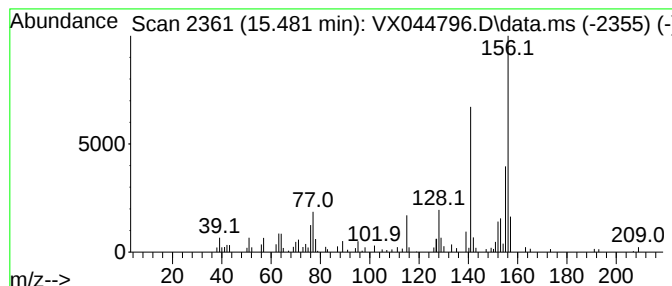
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012825WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Naphthalene, 2,7-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.481	2.60 ug/L	37577	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	95
2			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	94
3			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	93
4			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	93
5			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	93



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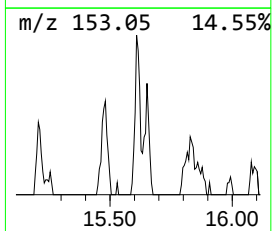
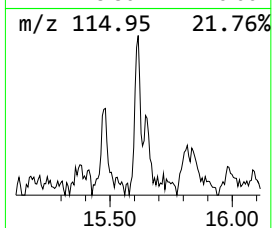
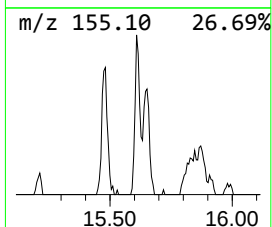
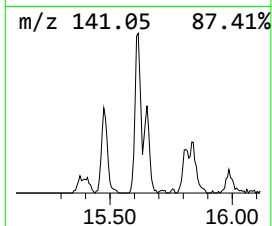
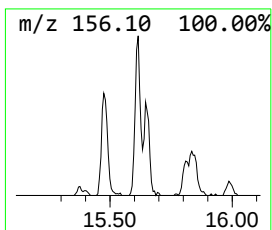
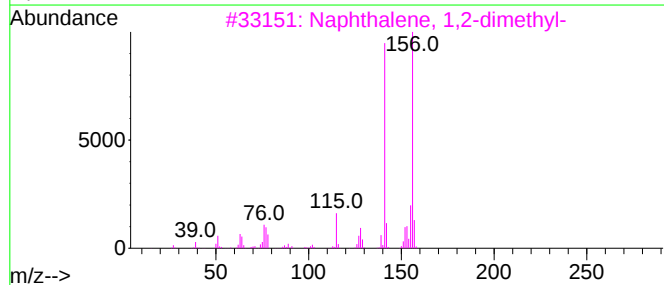
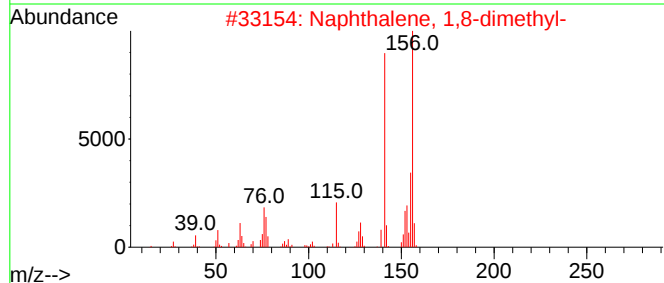
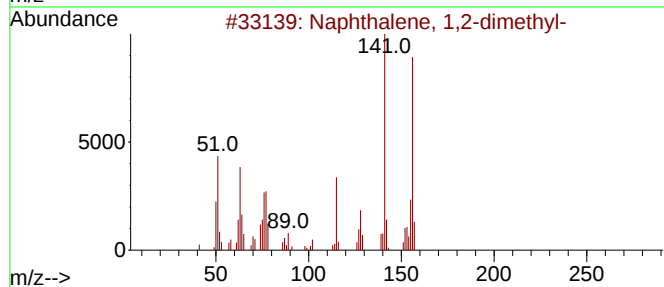
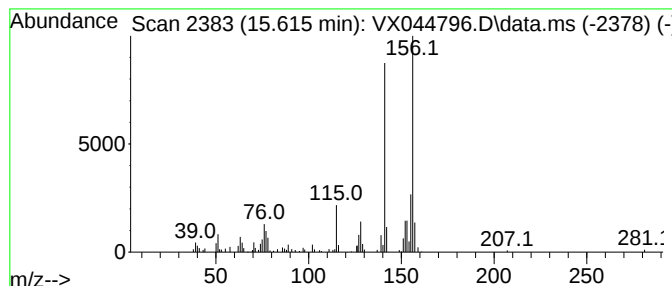
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012825WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Naphthalene, 1,2-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	3.21 ug/L	46334	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	97
2			Naphthalene, 1,8-dimethyl-	156	C12H12	000569-41-5	96
3			Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	96
4			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	96
5			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	95



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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
Naphthalene, 2,...	15.481	2.6	ug/L	37577	3	12.018	721338	50.0
Naphthalene, 1,...	15.615	3.2	ug/L	46334	3	12.018	721338	50.0