

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012825\
 Data File : VX044753.D
 Acq On : 28 Jan 2025 18:40
 Operator : JC/MD
 Sample : Q1148-05
 Misc : 10.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 XA174

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: VX044753.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	12	rBV	3329	3204	0.07%	0.007%
2	1.258	22	28	33	rBV2	11104	21796	0.45%	0.044%
3	1.368	42	46	50	rBV	63904	77631	1.61%	0.158%
4	1.648	72	92	95	rBV3	21400	73432	1.52%	0.150%
5	2.276	189	195	207	rBV	197000	312881	6.50%	0.637%
6	2.410	211	217	242	rVB	195589	482946	10.03%	0.984%
7	2.715	262	267	271	rBV	20399	36962	0.77%	0.075%
8	2.776	271	277	301	rVB	280716	693770	14.41%	1.413%
9	3.075	318	326	329	rBV	209999	391423	8.13%	0.797%
10	3.130	329	335	350	rVB	1037787	2386111	49.55%	4.860%
11	3.343	369	370	375	rVB3	592	659	0.01%	0.001%
12	3.416	378	382	389	rVB6	1478	3203	0.07%	0.007%
13	3.532	399	401	404	rVB4	477	593	0.01%	0.001%
14	3.843	449	452	454	rBV	466	568	0.01%	0.001%
15	4.117	492	497	498	rBV3	555	884	0.02%	0.002%
16	4.203	508	511	514	rBV2	532	641	0.01%	0.001%
17	4.483	545	557	567	rBV2	394532	1129182	23.45%	2.300%
18	4.904	622	626	633	rVB6	1634	3748	0.08%	0.008%
19	5.050	637	650	667	rBV	116577	367478	7.63%	0.748%
20	5.440	709	714	717	rBV3	708	1207	0.03%	0.002%
21	5.519	724	727	728	rBV	529	577	0.01%	0.001%
22	5.538	728	730	732	rBV	507	506	0.01%	0.001%
23	5.666	737	751	767	rBV	472725	1424294	29.58%	2.901%
24	5.958	788	799	804	rBV2	334401	947600	19.68%	1.930%
25	6.025	804	810	836	rVB2	1101578	3397263	70.54%	6.919%
26	6.379	866	868	872	rBV5	593	789	0.02%	0.002%
27	6.434	874	877	881	rVB3	501	710	0.01%	0.001%
28	6.476	881	884	885	rBV2	570	628	0.01%	0.001%
29	6.757	920	930	945	rBV	253438	619903	12.87%	1.263%
30	7.117	980	989	1004	rBV	904826	1978802	41.09%	4.030%
31	7.306	1011	1020	1038	rVB	191001	429018	8.91%	0.874%
32	7.428	1038	1040	1043	rBV3	626	701	0.01%	0.001%
33	7.574	1056	1064	1081	rBV	577547	1166144	24.21%	2.375%
34	7.818	1095	1104	1120	rBV	719765	1335742	27.74%	2.721%
35	7.970	1122	1129	1140	rVV	29257	60788	1.26%	0.124%
36	8.171	1157	1162	1164	rBV5	1259	2121	0.04%	0.004%

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37	8.324	1181	1187	1190	rBV	151701	250707	5.21%	0.511%
38	8.366	1190	1194	1206	rVB	336085	558003	11.59%	1.137%
39	8.519	1218	1219	1222	rBV3	669	641	0.01%	0.001%
40	8.580	1222	1229	1235	rVV	897183	1706419	35.43%	3.476%
41	8.647	1235	1240	1245	rVV	471024	781386	16.23%	1.591%
42	8.714	1245	1251	1272	rVB	1808317	2833464	58.84%	5.771%
43	8.952	1284	1290	1301	rBV	94739	152301	3.16%	0.310%
44	9.147	1316	1322	1336	rVV	1105061	1681745	34.92%	3.425%
45	9.269	1336	1342	1357	rVV	577041	854958	17.75%	1.741%
46	9.391	1357	1362	1365	rVV	192304	304722	6.33%	0.621%
47	9.433	1365	1369	1378	rVV	600386	1047870	21.76%	2.134%
48	9.519	1378	1383	1391	rVV	367053	531032	11.03%	1.082%
49	9.610	1391	1398	1410	rVB	609262	923273	19.17%	1.880%
50	9.848	1434	1437	1440	rVB4	537	646	0.01%	0.001%
51	9.970	1455	1457	1462	rVB4	515	574	0.01%	0.001%
52	10.055	1465	1471	1482	rBV	484037	722754	15.01%	1.472%
53	10.134	1482	1484	1488	rVV3	2261	3642	0.08%	0.007%
54	10.189	1488	1493	1506	rVV	2138611	2985282	61.99%	6.080%
55	10.299	1506	1511	1527	rVB	1398059	1980239	41.12%	4.033%
56	10.543	1549	1551	1556	rVB3	445	620	0.01%	0.001%
57	10.653	1561	1569	1587	rBV2	2733022	4815833	100.00%	9.809%
58	10.799	1587	1593	1603	rVB	447684	614186	12.75%	1.251%
59	10.963	1616	1620	1627	rVV2	5174	7903	0.16%	0.016%
60	11.018	1627	1629	1631	rVB2	778	763	0.02%	0.002%
61	11.098	1638	1642	1644	rBV3	840	1179	0.02%	0.002%
62	11.213	1652	1661	1663	rBV2	1172922	1951759	40.53%	3.975%
63	11.238	1663	1665	1674	rVV	664594	779975	16.20%	1.589%
64	11.311	1674	1677	1682	rVV5	3558	5285	0.11%	0.011%
65	11.378	1686	1688	1690	rBV3	688	600	0.01%	0.001%
66	11.451	1695	1700	1705	rBV3	2429	3709	0.08%	0.008%
67	11.488	1705	1706	1710	rVB3	791	863	0.02%	0.002%
68	11.719	1740	1744	1747	rBV2	7398	9624	0.20%	0.020%
69	11.750	1747	1749	1754	rVB2	3414	4181	0.09%	0.009%
70	11.860	1764	1767	1771	rBV4	421	742	0.02%	0.002%
71	11.969	1779	1785	1789	rBV	325345	412810	8.57%	0.841%
72	12.036	1789	1796	1807	rVB2	1320562	2267670	47.09%	4.619%
73	12.329	1837	1844	1863	rBV2	1589240	2543717	52.82%	5.181%
74	12.536	1874	1878	1883	rVB3	4062	5505	0.11%	0.011%
75	12.762	1909	1915	1919	rBV2	5250	7142	0.15%	0.015%
76	12.872	1927	1933	1935	rBV5	920	1661	0.03%	0.003%

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77	12.933	1940	1943	1946	rBV3	380	516	0.01%	0.001%
78	13.116	1967	1973	1977	rBV3	2932	4656	0.10%	0.009%
79	13.237	1990	1993	1995	rBV2	784	845	0.02%	0.002%
80	13.268	1995	1998	2003	rVV4	631	1132	0.02%	0.002%
81	13.353	2008	2012	2016	rVB3	282	517	0.01%	0.001%
82	13.591	2047	2051	2057	rVB3	5716	7966	0.17%	0.016%
83	13.774	2076	2081	2094	rBV	787728	950949	19.75%	1.937%
84	13.963	2107	2112	2117	rVV3	4509	5814	0.12%	0.012%
85	14.042	2122	2125	2127	rBV3	654	847	0.02%	0.002%
86	14.128	2136	2139	2146	rVV2	1782	2295	0.05%	0.005%
87	14.256	2157	2160	2163	rVB4	702	830	0.02%	0.002%
88	14.329	2170	2172	2177	rVB4	450	730	0.02%	0.001%
89	14.378	2177	2180	2182	rBV2	536	547	0.01%	0.001%
90	14.402	2182	2184	2188	rBV3	462	591	0.01%	0.001%
91	14.524	2201	2204	2209	rVB2	365	555	0.01%	0.001%
92	14.786	2245	2247	2250	rBV3	477	530	0.01%	0.001%
93	14.987	2277	2280	2282	rBV2	602	608	0.01%	0.001%
94	15.188	2310	2313	2315	rBV3	707	726	0.02%	0.001%
95	15.390	2341	2346	2350	rBV6	1182	2320	0.05%	0.005%
96	15.444	2352	2355	2357	rBV3	554	560	0.01%	0.001%
97	15.585	2374	2378	2380	rBV2	416	515	0.01%	0.001%
98	15.615	2381	2383	2386	rBV2	533	557	0.01%	0.001%
99	15.969	2434	2441	2445	rBV4	1624	3880	0.08%	0.008%
100	16.706	2561	2562	2564	rBV2	466	501	0.01%	0.001%

Sum of corrected areas: 49098277

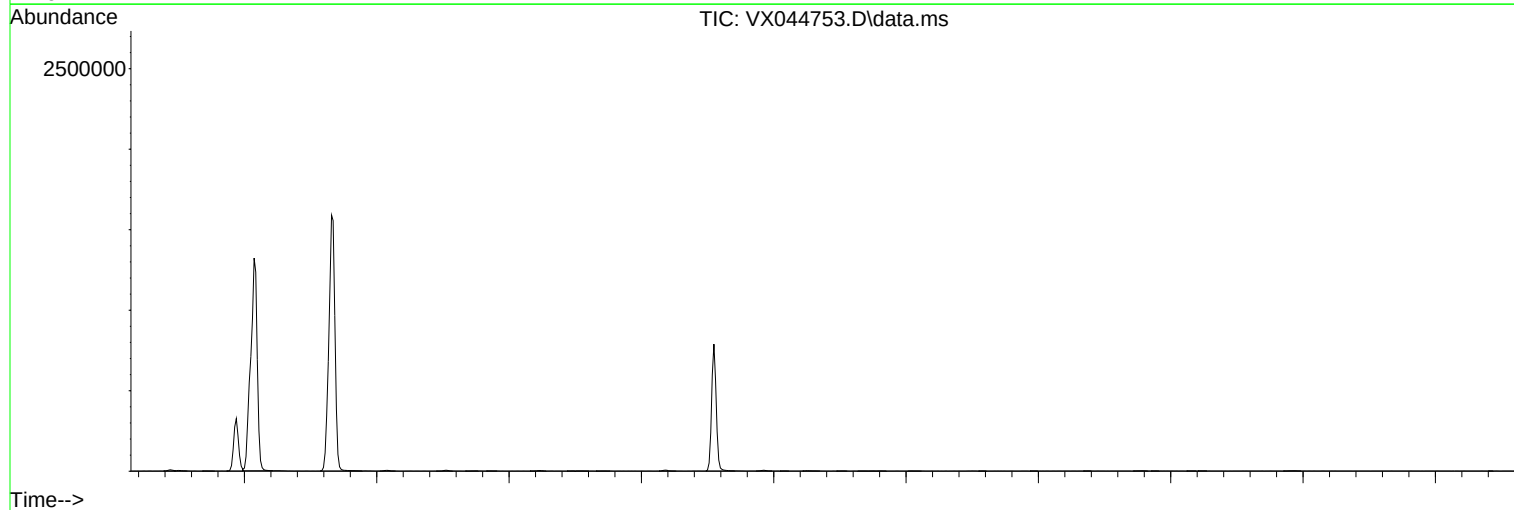
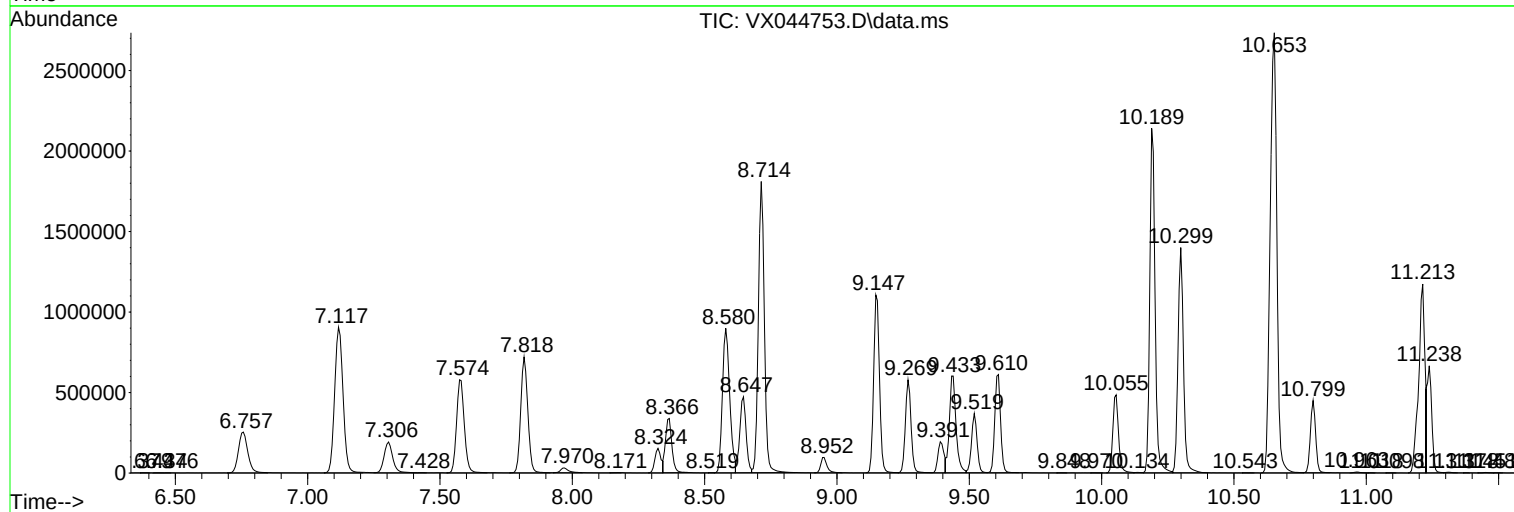
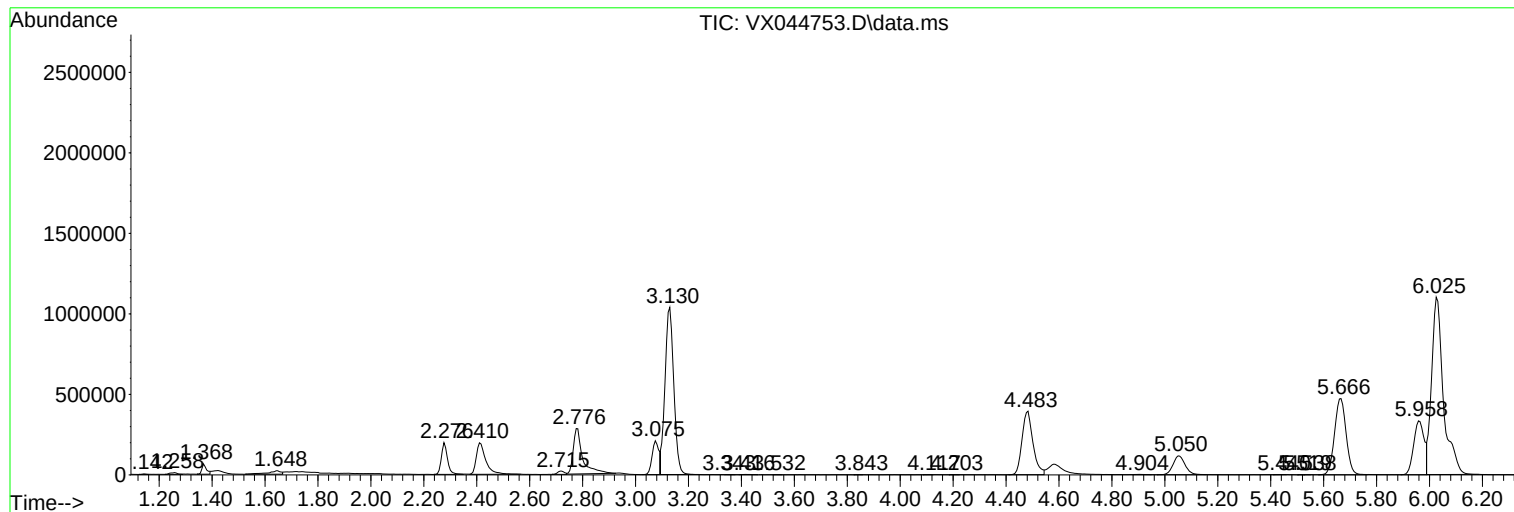
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ClientSampleId :
XA174

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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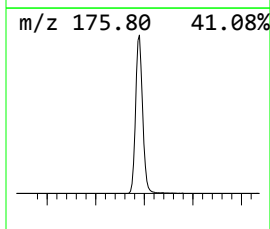
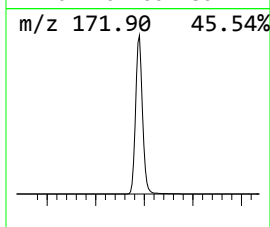
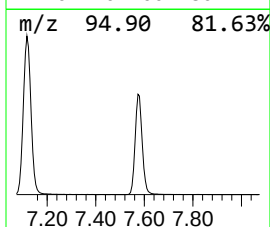
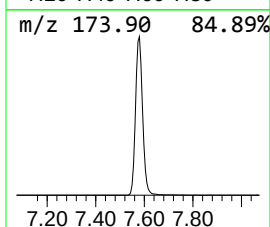
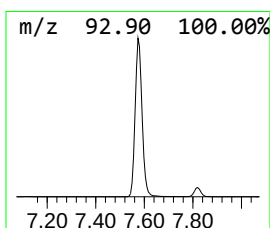
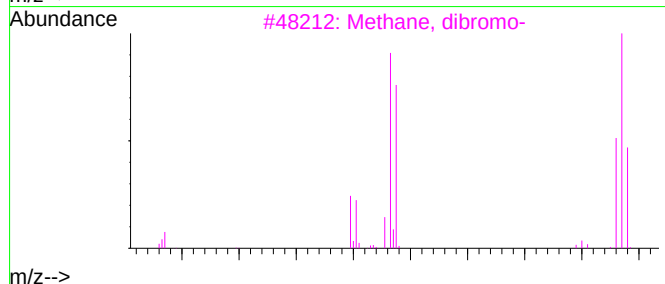
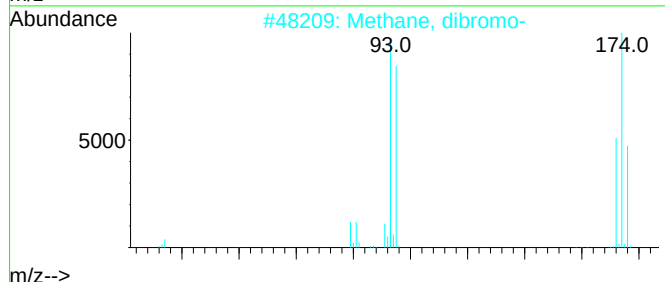
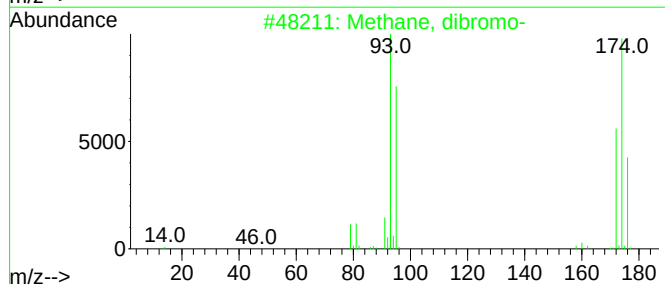
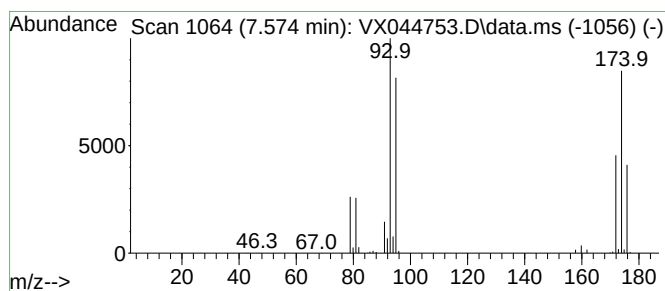
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM012825WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 Methane, dibromo- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
7.574	94.06 ug/L	1166140	1,4-Difluorobenzene	6.757	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methane, dibromo-	172	CH2Br2	000074-95-3	96
2	Methane, dibromo-	172	CH2Br2	000074-95-3	95
3	Methane, dibromo-	172	CH2Br2	000074-95-3	95
4	Methane, dibromo-	172	CH2Br2	000074-95-3	94
5	3-Chloro-6-methoxy-4-methylpyrid...	174	C6H7ClN2O2	050450-89-0	9



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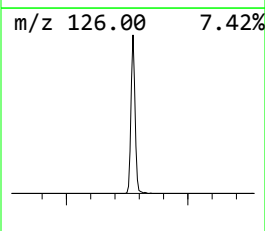
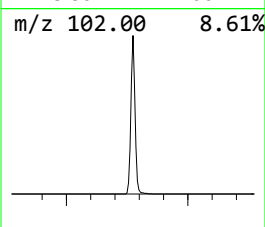
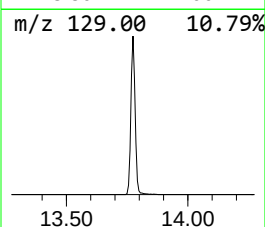
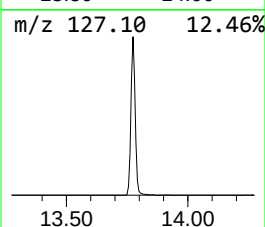
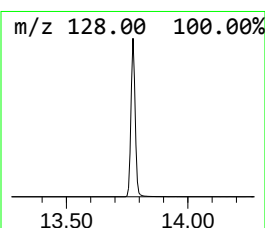
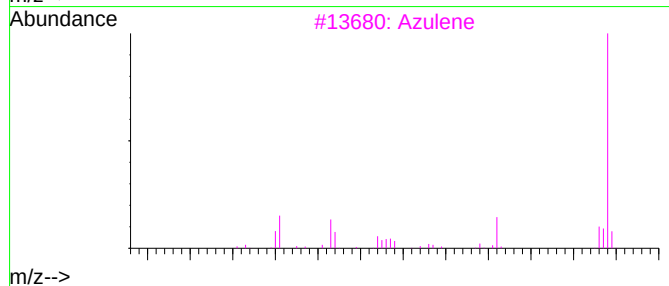
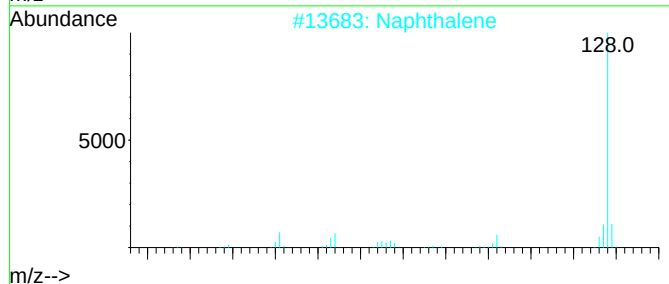
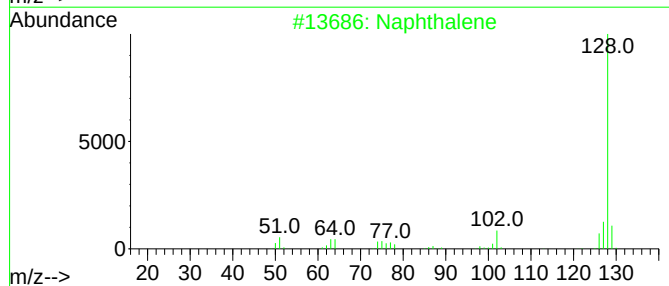
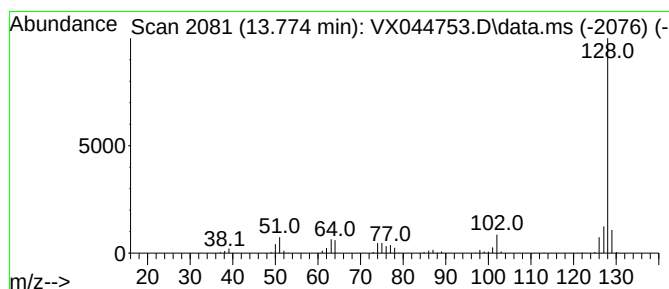
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 Azulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	20.97 ug/L	950949	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene	128	C10H8	000091-20-3	95
2	Naphthalene	128	C10H8	000091-20-3	93
3	Azulene	128	C10H8	000275-51-4	91
4	Azulene	128	C10H8	000275-51-4	91
5	Azulene	128	C10H8	000275-51-4	90



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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	#	RT	Resp	Conc
Methane, dibromo-	7.574	94.1	ug/L	1166140	1	6.757	619903	50.0
Azulene	13.774	21.0	ug/L	950949	3	12.024	2267670	50.0