

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012825\
 Data File : VX044746.D
 Acq On : 28 Jan 2025 15:58
 Operator : JC/MD
 Sample : Q1148-10
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 XA179

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

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: VX044746.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	rBV	14967	25024	1.19%	0.082%
2	1.368	42	46	62	rBV	136157	163820	7.80%	0.536%
3	1.642	88	91	102	rVB	55133	74970	3.57%	0.245%
4	1.874	123	129	141	rVB	160757	231353	11.02%	0.756%
5	2.300	192	199	207	rBV3	511485	971736	46.29%	3.177%
6	2.380	207	212	224	rVB	148920	253298	12.07%	0.828%
7	2.745	271	272	273	rBV	516	343	0.02%	0.001%
8	2.782	275	278	283	rVB4	1497	2207	0.11%	0.007%
9	2.818	283	284	286	rBV3	409	267	0.01%	0.001%
10	2.940	297	304	315	rVB	10030	22887	1.09%	0.075%
11	3.111	320	332	350	rBV2	719843	2099178	100.00%	6.863%
12	3.599	402	412	425	rBV	49714	121867	5.81%	0.398%
13	3.757	435	438	439	rBV2	417	340	0.02%	0.001%
14	3.776	439	441	443	rVB2	349	314	0.01%	0.001%
15	3.800	443	445	447	rVB	438	273	0.01%	0.001%
16	3.898	460	461	465	rBV	363	294	0.01%	0.001%
17	3.952	469	470	472	rVB	616	323	0.02%	0.001%
18	3.989	474	476	477	rBV	387	298	0.01%	0.001%
19	4.160	501	504	506	rBV2	428	571	0.03%	0.002%
20	4.196	506	510	511	rVV2	270	361	0.02%	0.001%
21	4.355	533	536	539	rBV2	428	558	0.03%	0.002%
22	4.477	545	556	571	rBV2	329323	998392	47.56%	3.264%
23	4.855	617	618	621	rBV2	396	320	0.02%	0.001%
24	4.934	627	631	632	rBV2	492	568	0.03%	0.002%
25	5.050	637	650	668	rBV	133465	419865	20.00%	1.373%
26	5.373	690	703	721	rVV	174963	555896	26.48%	1.817%
27	5.525	727	728	729	rBV	553	306	0.01%	0.001%
28	5.666	740	751	769	rVB	58388	174351	8.31%	0.570%
29	5.781	769	770	773	rBV	411	368	0.02%	0.001%
30	5.958	787	799	805	rBV3	369726	1105196	52.65%	3.613%
31	6.464	881	882	884	rBV2	627	407	0.02%	0.001%
32	6.623	905	908	909	rBV2	464	452	0.02%	0.001%
33	6.751	920	929	945	rBV	295759	734524	34.99%	2.401%
34	7.117	980	989	1011	rBV	463131	1013585	48.28%	3.314%
35	7.299	1011	1019	1032	rVV	222333	492025	23.44%	1.609%
36	7.421	1032	1039	1058	rVB	216294	469391	22.36%	1.535%

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37	7.696	1083	1084	1088	rVB2	629	691	0.03%	0.002%
38	7.818	1102	1104	1108	rBV3	562	810	0.04%	0.003%
39	7.872	1111	1113	1114	rBV	285	248	0.01%	0.001%
40	7.958	1123	1127	1132	rBV3	494	1097	0.05%	0.004%
41	8.007	1132	1135	1136	rBV2	557	677	0.03%	0.002%
42	8.257	1174	1176	1180	rBV2	450	501	0.02%	0.002%
43	8.324	1180	1187	1204	rBV	158160	286460	13.65%	0.937%
44	8.494	1210	1215	1221	rBV	31121	55476	2.64%	0.181%
45	8.567	1222	1227	1234	rVV	469258	778515	37.09%	2.545%
46	8.647	1234	1240	1246	rVV	517219	888360	42.32%	2.904%
47	8.714	1246	1251	1280	rVB	607349	1011022	48.16%	3.305%
48	8.976	1284	1294	1313	rBV2	596881	1079657	51.43%	3.530%
49	9.147	1316	1322	1335	rBV	593945	863203	41.12%	2.822%
50	9.269	1336	1342	1356	rVB	347788	512243	24.40%	1.675%
51	9.384	1356	1361	1377	rBV2	242187	377606	17.99%	1.234%
52	9.519	1377	1383	1392	rVB	529007	802598	38.23%	2.624%
53	9.695	1408	1412	1418	rBV6	1897	3348	0.16%	0.011%
54	9.927	1448	1450	1451	rBV	467	320	0.02%	0.001%
55	10.049	1465	1470	1488	rBV	596598	853922	40.68%	2.792%
56	10.299	1505	1511	1526	rBV	837993	1186492	56.52%	3.879%
57	10.652	1561	1569	1586	rBV2	1101683	1981338	94.39%	6.478%
58	10.799	1588	1593	1600	rVB	51536	72884	3.47%	0.238%
59	10.927	1612	1614	1616	rBV	447	338	0.02%	0.001%
60	10.963	1616	1620	1624	rVB4	1978	3010	0.14%	0.010%
61	11.091	1637	1641	1643	rBV3	526	620	0.03%	0.002%
62	11.189	1652	1657	1662	rBV2	377533	751314	35.79%	2.456%
63	11.238	1662	1665	1672	rVB	352477	452218	21.54%	1.478%
64	11.384	1685	1689	1694	rBV4	1976	2850	0.14%	0.009%
65	11.451	1694	1700	1712	rVV	911487	1141731	54.39%	3.733%
66	11.610	1723	1726	1733	rVB3	5585	8031	0.38%	0.026%
67	11.750	1744	1749	1761	rVB	1300200	1512409	72.05%	4.944%
68	11.969	1779	1785	1789	rBV	469852	612407	29.17%	2.002%
69	12.036	1789	1796	1809	rVB2	843479	1727299	82.28%	5.647%
70	12.274	1833	1835	1837	rBV2	426	567	0.03%	0.002%
71	12.317	1837	1842	1853	rVV3	555779	881625	42.00%	2.882%
72	12.487	1869	1870	1872	rVB	534	338	0.02%	0.001%
73	12.536	1874	1878	1884	rVB4	5813	8244	0.39%	0.027%
74	12.585	1884	1886	1888	rBV2	302	289	0.01%	0.001%
75	12.628	1888	1893	1894	rBV2	243	346	0.02%	0.001%
76	12.713	1904	1907	1908	rBV2	269	259	0.01%	0.001%

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Stop Thrs : 0

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77	12.756	1912	1914	1919	rVB3	933	1189	0.06%	0.004%
78	12.878	1933	1934	1936	rBV	290	246	0.01%	0.001%
79	12.957	1946	1947	1949	rBV2	370	250	0.01%	0.001%
80	13.122	1971	1974	1980	rVB3	609	935	0.04%	0.003%
81	13.329	2006	2008	2010	rVB2	408	327	0.02%	0.001%
82	13.396	2016	2019	2022	rVV3	229	263	0.01%	0.001%
83	13.475	2029	2032	2033	rBV2	377	405	0.02%	0.001%
84	13.530	2040	2041	2043	rBV2	397	278	0.01%	0.001%
85	13.585	2044	2050	2061	rVV	448494	550063	26.20%	1.798%
86	13.725	2067	2073	2077	rBV	457087	589785	28.10%	1.928%
87	13.774	2077	2081	2094	rVB	1349785	1636325	77.95%	5.350%
88	13.963	2109	2112	2116	rVB2	2697	3293	0.16%	0.011%
89	14.066	2128	2129	2130	rBV	417	275	0.01%	0.001%
90	14.127	2135	2139	2144	rVB2	1973	2692	0.13%	0.009%
91	14.213	2151	2153	2157	rVB3	383	492	0.02%	0.002%
92	14.365	2175	2178	2179	rBV2	366	370	0.02%	0.001%
93	14.444	2189	2191	2193	rBV	348	312	0.01%	0.001%
94	14.518	2200	2203	2204	rBV3	580	492	0.02%	0.002%
95	14.719	2233	2236	2237	rBV2	372	298	0.01%	0.001%
96	14.774	2244	2245	2247	rBV2	259	248	0.01%	0.001%
97	15.066	2291	2293	2295	rBV	640	555	0.03%	0.002%
98	15.158	2306	2308	2312	rBV2	611	811	0.04%	0.003%
99	15.219	2316	2318	2320	rVV2	580	380	0.02%	0.001%
100	16.651	2551	2553	2555	rBV2	438	395	0.02%	0.001%

Sum of corrected areas: 30587970

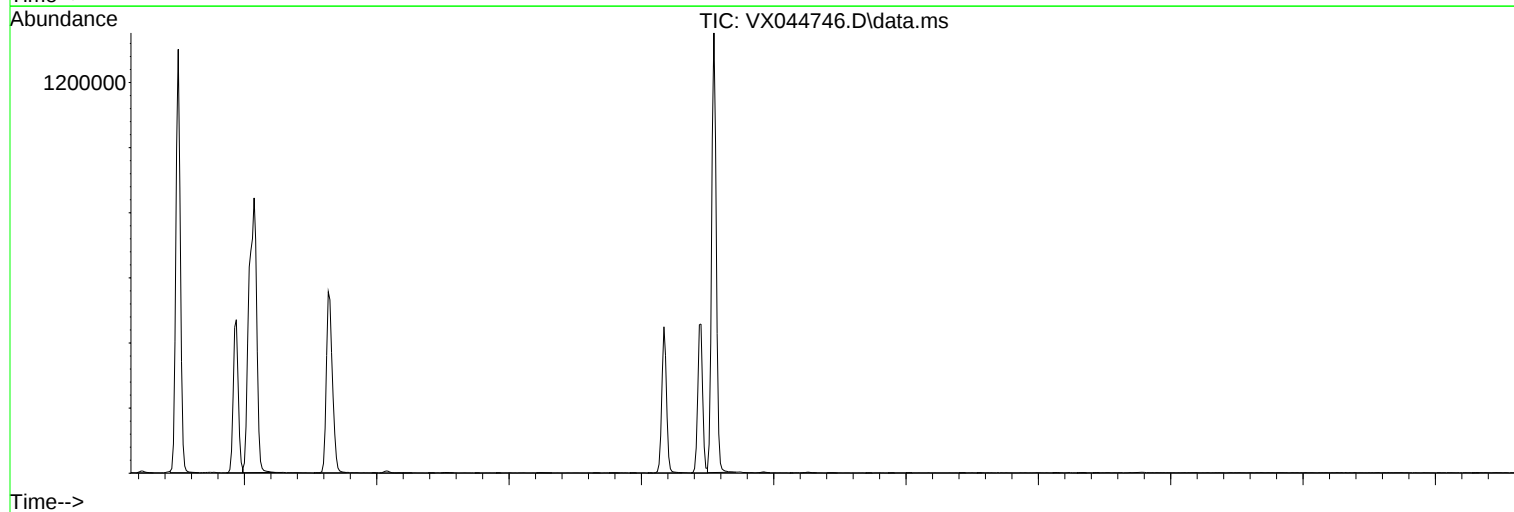
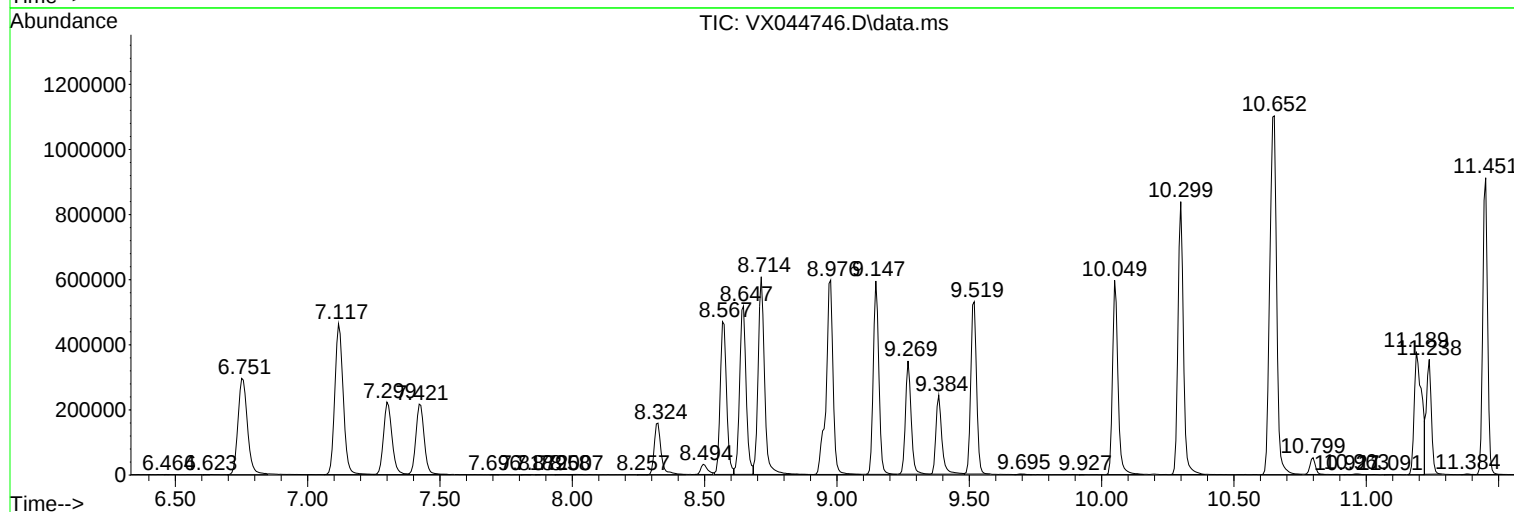
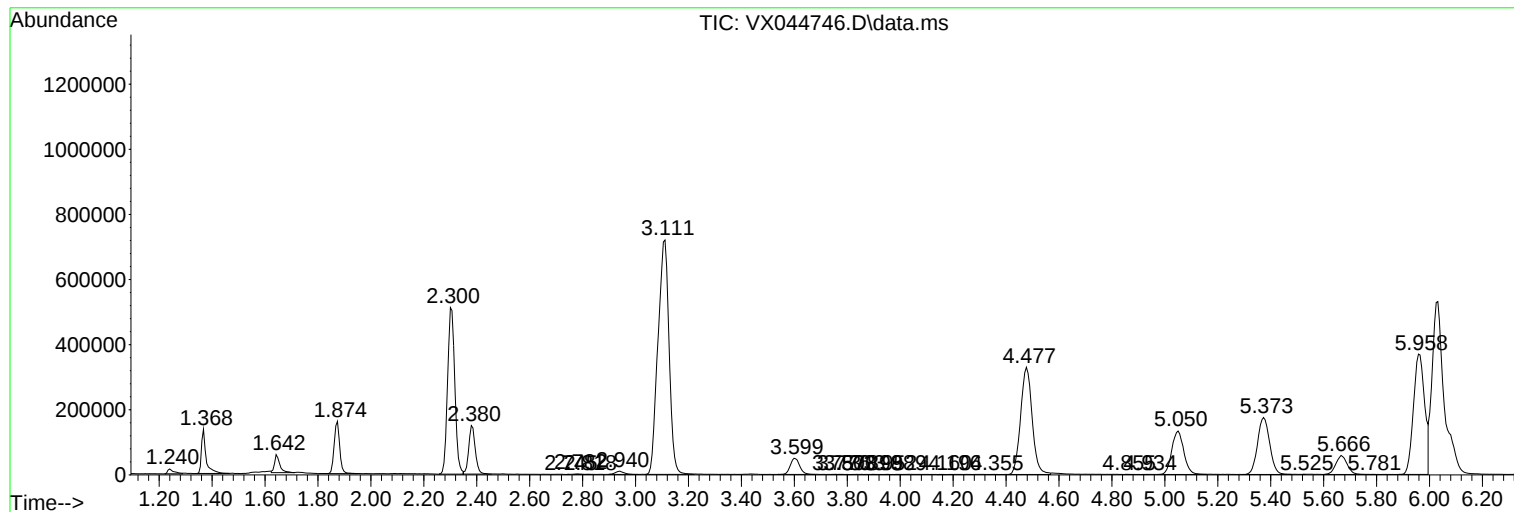
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012825WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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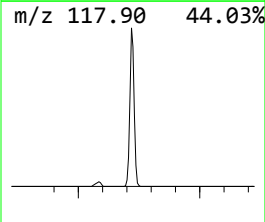
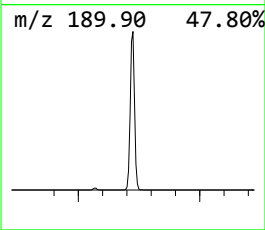
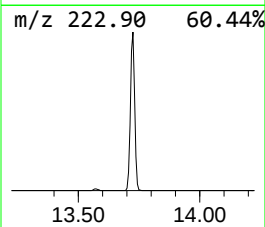
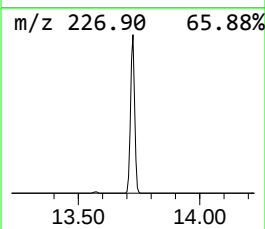
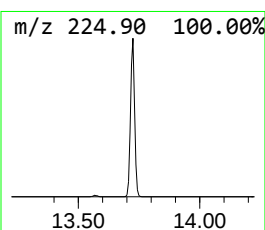
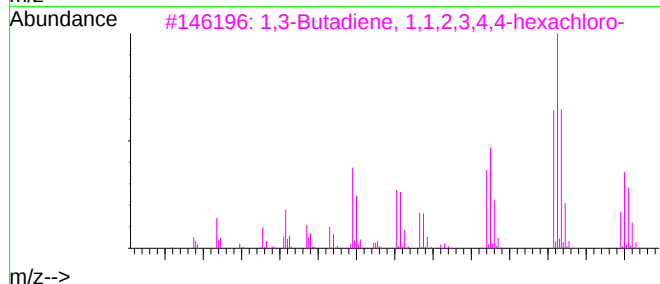
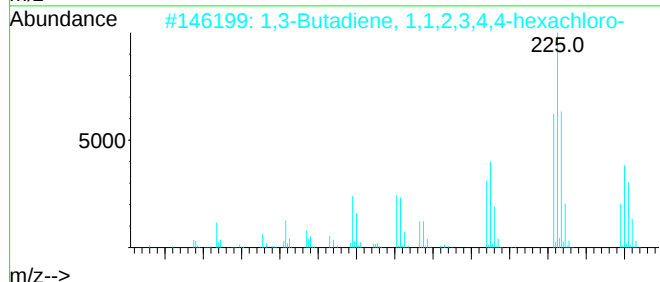
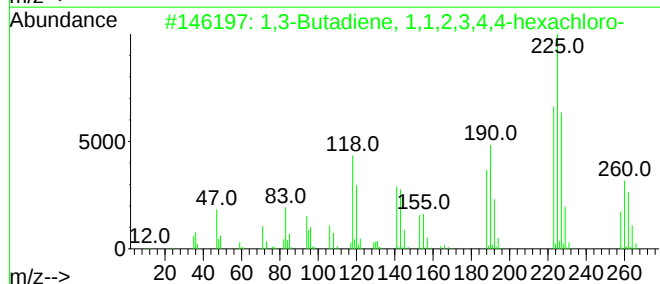
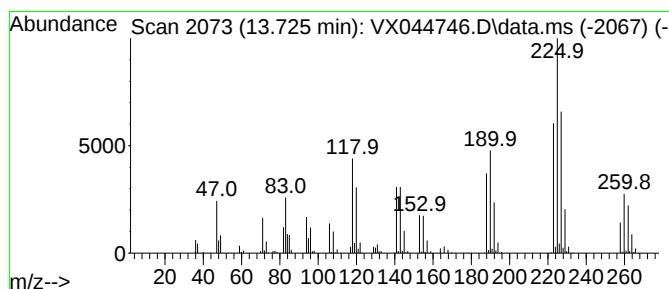
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.725	17.07 ug/L	589785	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	99
2			1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	99
3			1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	99
4			1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	99
5			Tin(IV) chloride	260	Cl4Sn	007646-78-8	43



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Quant Title : VOC Analysis

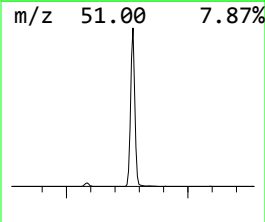
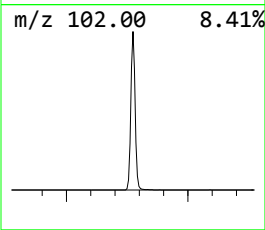
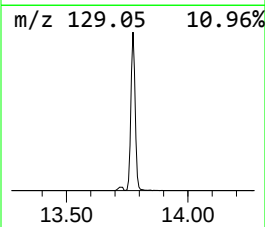
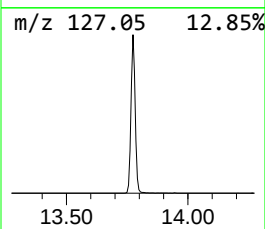
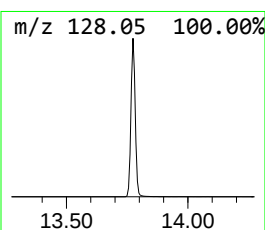
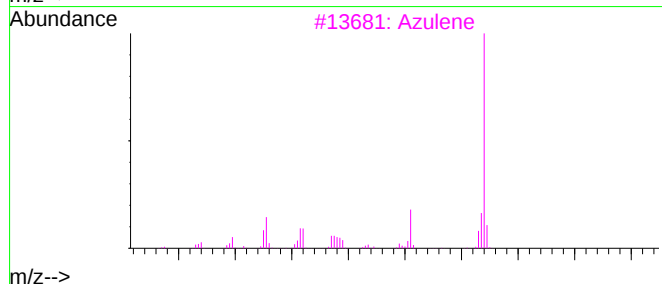
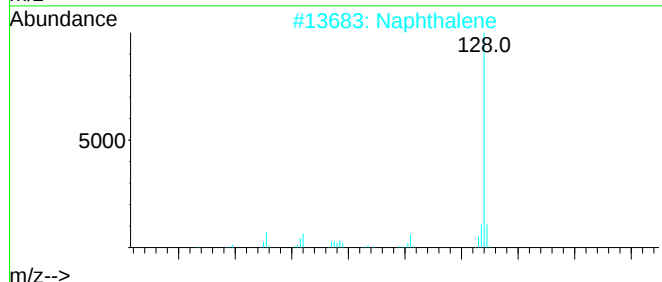
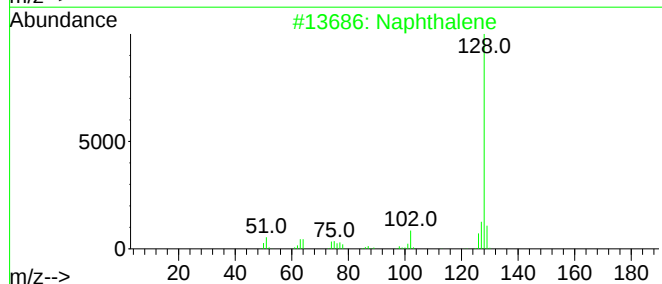
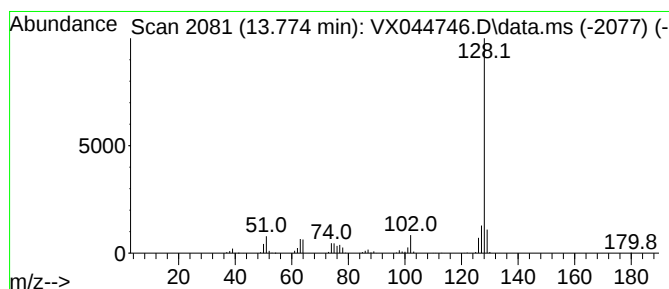
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	47.37 ug/L	1636330	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene	128	C10H8	000091-20-3	95
2	Naphthalene	128	C10H8	000091-20-3	94
3	Azulene	128	C10H8	000275-51-4	91
4	Naphthalene	128	C10H8	000091-20-3	91
5	Azulene	128	C10H8	000275-51-4	91



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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
1,3-Butadiene, ...	13.725	17.1	ug/L	589785	3	12.018	1727300	50.0
Azulene	13.774	47.4	ug/L	1636330	3	12.018	1727300	50.0