

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU013025\
 Data File : VU063104.D
 Acq On : 30 Jan 2025 17:36
 Operator : MD/SY
 Sample : Q1148-10
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 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_U\Method\SFAMULM013025WMA.M
 Title : VOC Analysis

Signal : TIC: VU063104.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.592	85	94	111	rVB	76082	90277	8.54%	0.557%
2	1.895	180	188	205	rVB	44096	60182	5.69%	0.371%
3	2.126	250	260	276	rBV	85569	126287	11.95%	0.779%
4	2.222	287	290	294	rVV	220	181	0.02%	0.001%
5	2.322	317	321	326	rBV	227	276	0.03%	0.002%
6	2.357	326	332	336	rVV2	338	295	0.03%	0.002%
7	2.406	343	347	348	rBV	188	154	0.01%	0.001%
8	2.448	358	360	363	rBV2	179	138	0.01%	0.001%
9	2.563	381	396	405	rBV3	271249	527269	49.88%	3.252%
10	2.611	405	411	434	rVB	79980	136263	12.89%	0.840%
11	2.782	460	464	474	rVB2	2025	2708	0.26%	0.017%
12	2.936	508	512	518	rBV2	209	328	0.03%	0.002%
13	3.023	536	539	540	rBV	410	195	0.02%	0.001%
14	3.168	573	584	600	rBV2	4032	9497	0.90%	0.059%
15	3.345	622	639	676	rBV2	424645	980542	92.77%	6.048%
16	3.611	720	722	726	rVV	211	154	0.01%	0.001%
17	3.685	729	745	760	rVV4	4821	10660	1.01%	0.066%
18	3.853	783	797	817	rBV	23539	55252	5.23%	0.341%
19	4.017	842	848	854	rBV2	157	241	0.02%	0.001%
20	4.213	907	909	913	rBV	181	165	0.02%	0.001%
21	4.309	935	939	941	rBV2	175	147	0.01%	0.001%
22	4.570	1017	1020	1022	rBV	192	161	0.02%	0.001%
23	4.608	1022	1032	1034	rBV	56275	79397	7.51%	0.490%
24	4.859	1108	1110	1115	rVB3	262	191	0.02%	0.001%
25	4.901	1119	1123	1128	rVB3	340	372	0.04%	0.002%
26	4.939	1133	1135	1140	rVB2	392	315	0.03%	0.002%
27	4.975	1141	1146	1148	rBV2	393	382	0.04%	0.002%
28	5.045	1154	1168	1194	rBV	97065	214918	20.33%	1.326%
29	5.168	1202	1206	1208	rBV	182	142	0.01%	0.001%
30	5.300	1231	1247	1268	rBV2	129404	294461	27.86%	1.816%
31	5.390	1272	1275	1279	rVB2	381	248	0.02%	0.002%
32	5.509	1298	1312	1332	rBV3	37258	83716	7.92%	0.516%
33	5.711	1356	1375	1382	rBV2	208983	550212	52.05%	3.394%
34	5.759	1384	1390	1427	rVB2	356258	773565	73.18%	4.771%
35	6.235	1526	1538	1561	rBV	173377	331244	31.34%	2.043%
36	6.476	1610	1613	1616	rVB	278	161	0.02%	0.001%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM013025WMA.M
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37	6.528	1616	1629	1654	rBV	269039	504749	47.75%	3.113%
38	6.676	1663	1675	1694	rBV	124691	241844	22.88%	1.492%
39	6.779	1694	1707	1731	rVB	110545	212538	20.11%	1.311%
40	6.865	1731	1734	1737	rBV3	276	161	0.02%	0.001%
41	6.933	1752	1755	1760	rVB2	215	169	0.02%	0.001%
42	7.187	1828	1834	1837	rBV2	370	378	0.04%	0.002%
43	7.235	1847	1849	1855	rBV	209	253	0.02%	0.002%
44	7.479	1922	1925	1928	rBV2	184	175	0.02%	0.001%
45	7.553	1934	1948	1970	rBV	71850	131390	12.43%	0.810%
46	7.708	1987	1996	2007	rVV	13353	23122	2.19%	0.143%
47	7.775	2007	2017	2038	rVV	213240	370539	35.06%	2.285%
48	7.885	2040	2051	2064	rVV	263329	455356	43.08%	2.809%
49	7.959	2064	2074	2102	rVB	319540	548689	51.91%	3.384%
50	8.119	2121	2124	2127	rVB2	390	211	0.02%	0.001%
51	8.196	2128	2148	2172	rBV2	248686	498603	47.17%	3.075%
52	8.328	2187	2189	2195	rVB	216	169	0.02%	0.001%
53	8.386	2195	2207	2232	rBV	259165	439005	41.53%	2.708%
54	8.489	2237	2239	2244	rVB2	396	210	0.02%	0.001%
55	8.541	2244	2255	2270	rBV	154580	264542	25.03%	1.632%
56	8.621	2270	2280	2311	rBV	152361	266695	25.23%	1.645%
57	8.798	2322	2335	2359	rVB	235700	402256	38.06%	2.481%
58	8.914	2369	2371	2375	rVB	438	218	0.02%	0.001%
59	8.942	2378	2380	2383	rVB	264	144	0.01%	0.001%
60	9.029	2404	2407	2412	rBV2	232	203	0.02%	0.001%
61	9.052	2412	2414	2418	rVB	184	139	0.01%	0.001%
62	9.106	2427	2431	2434	rBV2	198	194	0.02%	0.001%
63	9.405	2512	2524	2546	rBV	253191	423995	40.11%	2.615%
64	9.499	2551	2553	2560	rVV3	674	835	0.08%	0.005%
65	9.566	2569	2574	2584	rVB3	826	1184	0.11%	0.007%
66	9.634	2592	2595	2598	rBV2	183	139	0.01%	0.001%
67	9.682	2598	2610	2641	rVV	353004	584352	55.28%	3.604%
68	9.830	2653	2656	2659	rVB2	263	152	0.01%	0.001%
69	9.849	2659	2662	2664	rBV2	204	166	0.02%	0.001%
70	10.036	2717	2720	2725	rBV2	159	177	0.02%	0.001%
71	10.100	2725	2740	2778	rVV3	502489	992019	93.85%	6.119%
72	10.280	2786	2796	2808	rVB	25105	41007	3.88%	0.253%
73	10.479	2850	2858	2865	rBV3	1171	1637	0.15%	0.010%
74	10.547	2875	2879	2882	rBV2	197	209	0.02%	0.001%
75	10.743	2926	2940	2954	rBV2	196915	480910	45.50%	2.966%
76	10.811	2955	2961	2980	rVB	153135	244109	23.09%	1.506%

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 Title : VOC Analysis

77	10.987	3012	3016	3017	rBV2	522	372	0.04%	0.002%
78	11.077	3030	3044	3070	rBV	410253	616923	58.37%	3.805%
79	11.286	3101	3109	3126	rVB2	2204	3258	0.31%	0.020%
80	11.457	3142	3162	3181	rBV	557798	850839	80.50%	5.248%
81	11.573	3196	3198	3201	rBV2	222	179	0.02%	0.001%
82	11.602	3205	3207	3211	rVB2	323	218	0.02%	0.001%
83	11.733	3237	3248	3259	rBV	230776	367891	34.80%	2.269%
84	11.823	3259	3276	3307	rVB2	408826	1057007	100.00%	6.519%
85	12.183	3376	3388	3411	rBV2	280837	560975	53.07%	3.460%
86	12.466	3467	3476	3488	rVB6	1795	2688	0.25%	0.017%
87	13.081	3664	3667	3670	rBV2	245	227	0.02%	0.001%
88	13.129	3677	3682	3685	rBV2	212	258	0.02%	0.002%
89	13.225	3704	3712	3720	rBV4	1204	1777	0.17%	0.011%
90	13.302	3730	3736	3739	rVB3	250	270	0.03%	0.002%
91	13.380	3757	3760	3766	rVB3	225	271	0.03%	0.002%
92	13.450	3779	3782	3790	rVB3	257	243	0.02%	0.001%
93	13.482	3790	3792	3795	rBV	233	167	0.02%	0.001%
94	13.830	3888	3900	3915	rBV	167807	263931	24.97%	1.628%
95	14.010	3945	3956	3966	rBV2	202919	313704	29.68%	1.935%
96	14.077	3966	3977	4010	rVB	424470	704232	66.63%	4.344%
97	14.322	4047	4053	4061	rVB5	2257	3121	0.30%	0.019%
98	14.569	4127	4130	4132	rBV2	254	174	0.02%	0.001%
99	15.206	4325	4328	4331	rBV4	309	274	0.03%	0.002%
100	15.338	4364	4369	4373	rBV4	349	516	0.05%	0.003%

Sum of corrected areas: 16213054

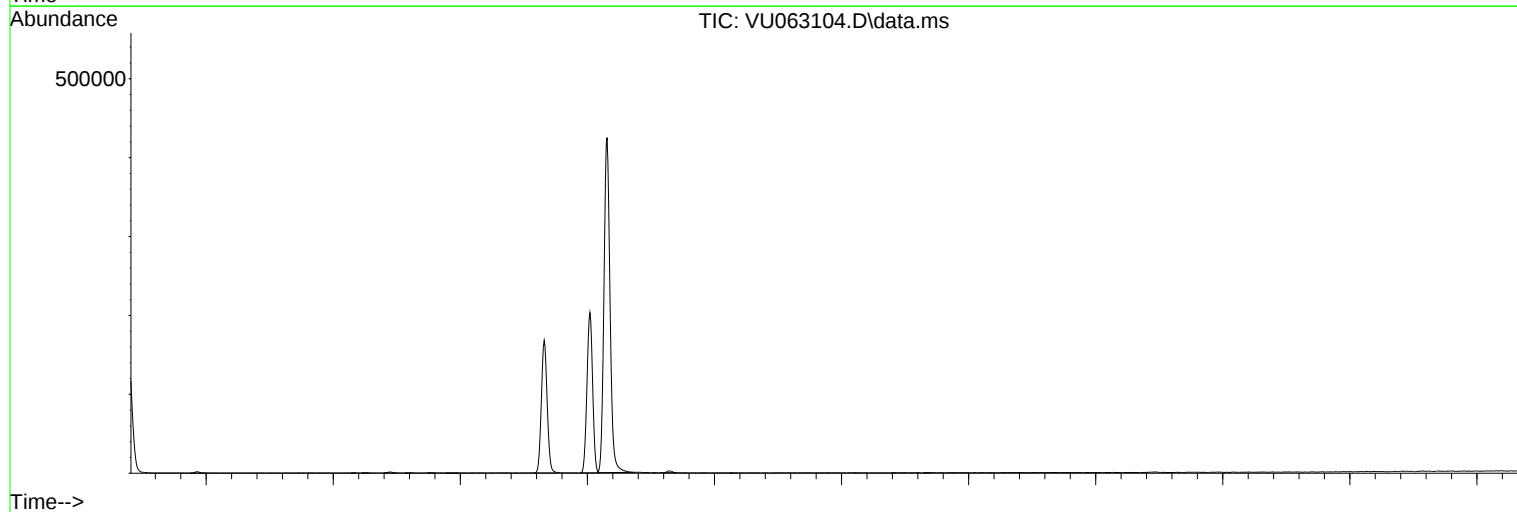
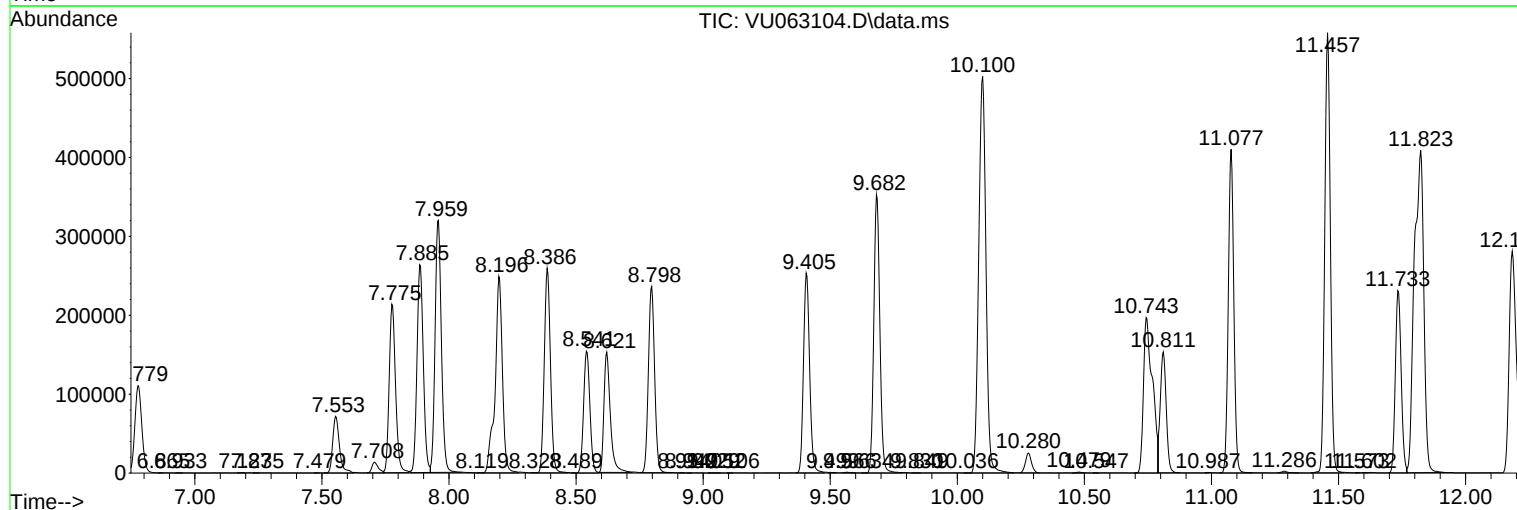
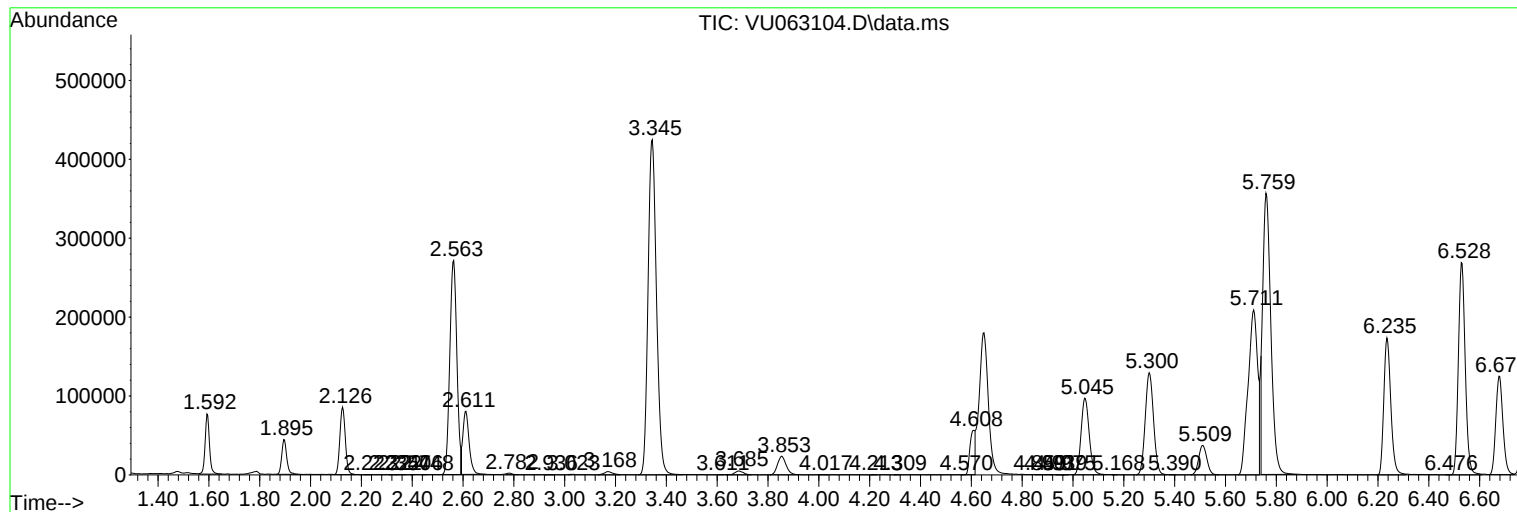
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM013025WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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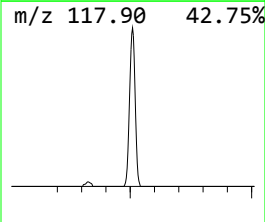
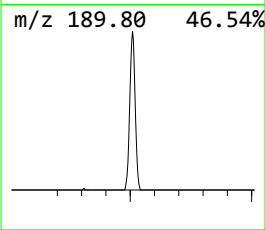
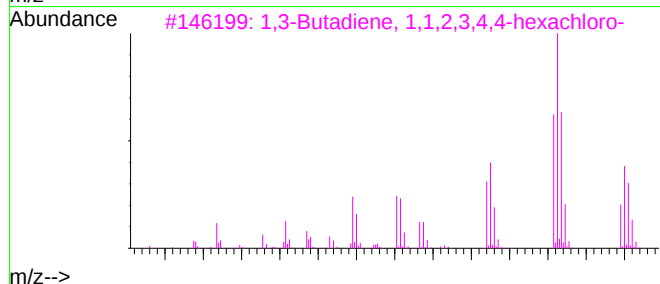
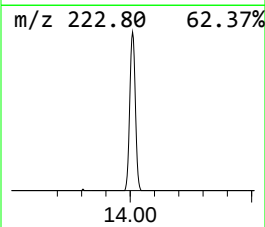
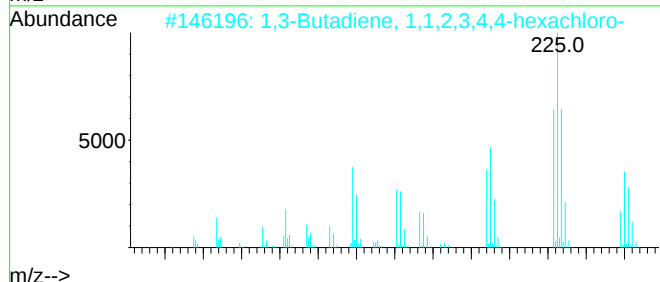
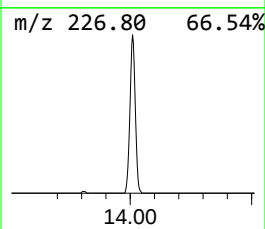
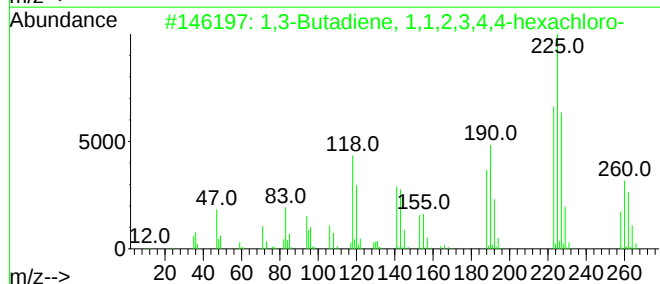
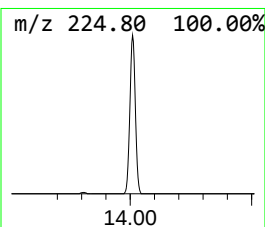
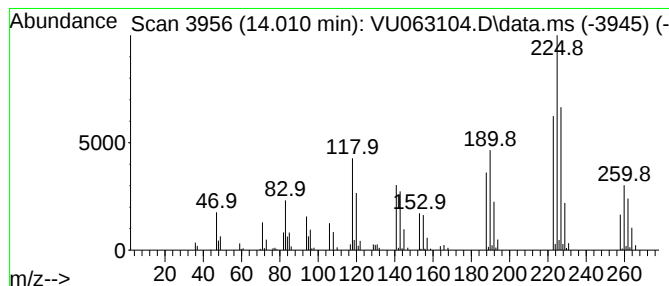
TIC Library : C:\Database\NIST20.L

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.
14.010	14.84 ug/L	313704	1,4-Dichlorobenzene-d4	11.801

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	98
5	Tin(IV) chloride		260	Cl4Sn	007646-78-8	37



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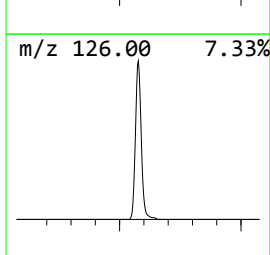
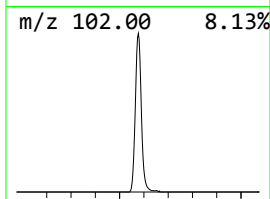
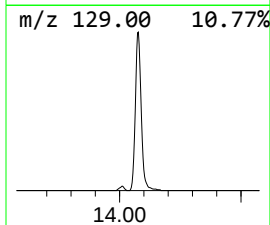
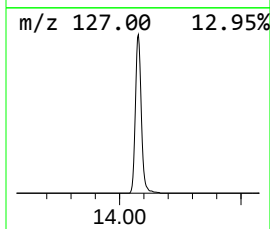
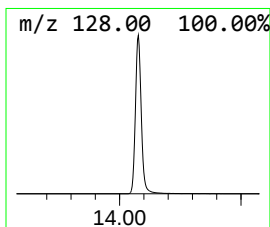
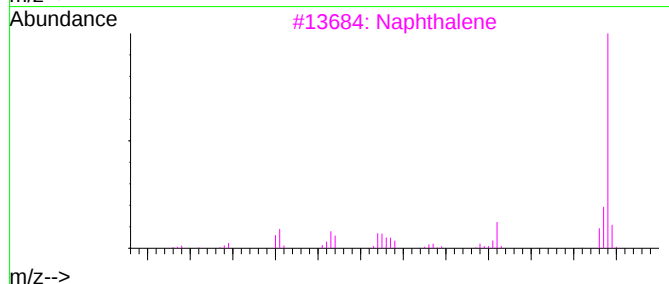
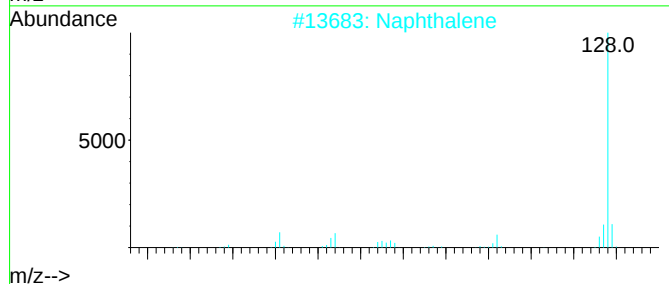
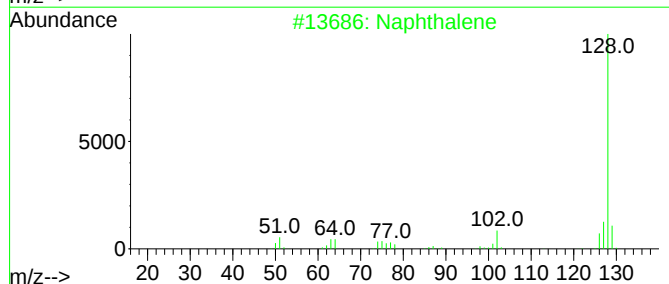
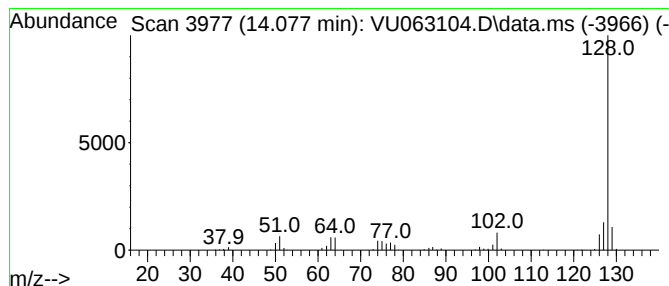
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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.077	33.31 ug/L	704232	1,4-Dichlorobenzene-d4		11.801	
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	Naphthalene		128	C10H8	000091-20-3	94
4	Azulene		128	C10H8	000275-51-4	93
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, ...	14.010	14.8	ug/L	313704	3	11.801	1057010	50.0
Azulene	14.077	33.3	ug/L	704232	3	11.801	1057010	50.0