

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120221\
 Data File : VU046055.D
 Acq On : 02 Dec 2021 16:19
 Operator : SY/MD
 Sample : M4870-05
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGKP2

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_U\Method\SFAMULM112921WMA.M
 Title : VOC Analysis

Signal : TIC: VU046055.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.600	73	81	93	rVB	94394	103624	13.13%	1.472%
2	1.703	105	113	125	rBV3	3702	7689	0.97%	0.109%
3	1.916	171	179	191	rVB	72043	92274	11.70%	1.311%
4	2.572	368	383	397	rBV	158025	264522	33.53%	3.757%
5	2.649	399	407	430	rVV	13485	33410	4.23%	0.475%
6	2.800	446	454	459	rVB	512	693	0.09%	0.010%
7	2.961	498	504	507	rBV2	333	381	0.05%	0.005%
8	3.051	522	532	544	rVB2	7612	13416	1.70%	0.191%
9	3.186	564	574	577	rBV2	757	1189	0.15%	0.017%
10	3.420	645	647	651	rBV	159	153	0.02%	0.002%
11	3.501	669	672	676	rBB	140	146	0.02%	0.002%
12	3.549	681	687	689	rBV	167	220	0.03%	0.003%
13	3.578	689	696	697	rBV2	963	921	0.12%	0.013%
14	3.858	780	783	787	rBB	181	163	0.02%	0.002%
15	3.880	788	790	796	rBB	132	165	0.02%	0.002%
16	4.076	848	851	855	rBB	204	186	0.02%	0.003%
17	4.115	860	863	867	rBB	127	138	0.02%	0.002%
18	4.141	868	871	874	rBV	173	157	0.02%	0.002%
19	4.250	902	905	909	rBV	188	197	0.02%	0.003%
20	4.282	912	915	919	rBB	150	150	0.02%	0.002%
21	4.317	920	926	929	rBB	141	191	0.02%	0.003%
22	4.459	959	970	984	rVV3	2018	4382	0.56%	0.062%
23	4.562	999	1002	1005	rBV	274	268	0.03%	0.004%
24	4.633	1009	1024	1045	rBV	81619	217021	27.51%	3.083%
25	5.067	1143	1159	1179	rBV	140111	309763	39.26%	4.400%
26	5.198	1197	1200	1203	rVB	211	137	0.02%	0.002%
27	5.288	1225	1228	1230	rBV2	256	212	0.03%	0.003%
28	5.729	1343	1365	1384	rBV2	291586	788977	100.00%	11.207%
29	5.886	1411	1414	1419	rVB2	325	285	0.04%	0.004%
30	5.932	1426	1428	1432	rVB2	172	141	0.02%	0.002%
31	5.960	1434	1437	1439	rVV	367	301	0.04%	0.004%
32	5.986	1442	1445	1450	rVV2	288	324	0.04%	0.005%
33	6.009	1450	1452	1453	rVV	302	143	0.02%	0.002%
34	6.137	1489	1492	1493	rBV	382	169	0.02%	0.002%
35	6.250	1513	1527	1549	rBV	271454	513693	65.11%	7.297%
36	6.533	1605	1615	1629	rBV3	6114	13044	1.65%	0.185%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
 Title : VOC Analysis

37	6.694	1651	1665	1682	rBV	184576	353435	44.80%	5.020%
38	6.819	1702	1704	1709	rVB2	337	223	0.03%	0.003%
39	6.880	1717	1723	1733	rBV6	2345	3887	0.49%	0.055%
40	7.018	1762	1766	1768	rBV	154	158	0.02%	0.002%
41	7.044	1768	1774	1780	rVB2	494	687	0.09%	0.010%
42	7.076	1781	1784	1786	rBV	238	165	0.02%	0.002%
43	7.128	1797	1800	1801	rBV	321	172	0.02%	0.002%
44	7.182	1809	1817	1827	rVB3	1853	2966	0.38%	0.042%
45	7.224	1827	1830	1833	rVB	171	133	0.02%	0.002%
46	7.282	1843	1848	1850	rBV	166	188	0.02%	0.003%
47	7.349	1866	1869	1873	rVB	178	159	0.02%	0.002%
48	7.407	1885	1887	1892	rBV	131	159	0.02%	0.002%
49	7.568	1923	1937	1951	rBV	105373	179405	22.74%	2.548%
50	7.687	1968	1974	1984	rVB5	1303	1976	0.25%	0.028%
51	7.796	1998	2008	2019	rVB3	2278	3383	0.43%	0.048%
52	7.899	2025	2040	2057	rBV	368674	652412	82.69%	9.267%
53	8.038	2079	2083	2086	rBV2	517	427	0.05%	0.006%
54	8.182	2116	2128	2142	rVV	70993	116742	14.80%	1.658%
55	8.237	2142	2145	2155	rVV3	968	1329	0.17%	0.019%
56	8.288	2159	2161	2163	rVV3	250	133	0.02%	0.002%
57	8.314	2167	2169	2172	rVB	213	135	0.02%	0.002%
58	8.449	2208	2211	2214	rVB	173	136	0.02%	0.002%
59	8.475	2215	2219	2220	rBV	199	163	0.02%	0.002%
60	8.632	2256	2268	2301	rBV	253038	452439	57.35%	6.427%
61	8.787	2309	2316	2329	rVB5	6695	11628	1.47%	0.165%
62	8.870	2334	2342	2348	rVB4	974	1334	0.17%	0.019%
63	8.925	2348	2359	2367	rBV4	2042	3598	0.46%	0.051%
64	9.124	2416	2421	2426	rVV2	663	771	0.10%	0.011%
65	9.169	2426	2435	2443	rVV3	1428	1847	0.23%	0.026%
66	9.211	2443	2448	2453	rVB	587	577	0.07%	0.008%
67	9.337	2480	2487	2497	rBV3	1001	1478	0.19%	0.021%
68	9.420	2500	2513	2536	rBV	384688	651050	82.52%	9.248%
69	9.571	2550	2560	2577	rBV2	8230	12809	1.62%	0.182%
70	9.693	2584	2598	2613	rVV3	11497	23753	3.01%	0.337%
71	9.767	2613	2621	2634	rVB6	1440	3063	0.39%	0.044%
72	9.877	2651	2655	2656	rBV	394	248	0.03%	0.004%
73	9.890	2656	2659	2667	rVB2	661	606	0.08%	0.009%
74	9.947	2673	2677	2679	rBV2	404	353	0.04%	0.005%
75	10.021	2691	2700	2710	rBV9	5895	13182	1.67%	0.187%
76	10.115	2719	2729	2741	rVB7	5463	12293	1.56%	0.175%

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77	10.169	2743	2746	2755	rVB5	2882	3355	0.43%	0.048%
78	10.253	2755	2772	2785	rBV5	13018	26863	3.40%	0.382%
79	10.349	2786	2802	2811	rBV7	9718	21640	2.74%	0.307%
80	10.462	2828	2837	2838	rBV2	2307	2572	0.33%	0.037%
81	10.481	2840	2843	2852	rVB2	4126	5608	0.71%	0.080%
82	10.555	2852	2866	2876	rBV7	8363	18396	2.33%	0.261%
83	10.626	2881	2888	2894	rBV4	5079	6971	0.88%	0.099%
84	10.674	2897	2903	2914	rVB2	7804	11513	1.46%	0.164%
85	10.758	2917	2929	2940	rBV	266026	415229	52.63%	5.898%
86	11.378	3115	3122	3127	rBV3	10822	15967	2.02%	0.227%
87	11.417	3127	3134	3141	rVB2	35035	45874	5.81%	0.652%
88	11.465	3142	3149	3156	rBV4	14517	24457	3.10%	0.347%
89	11.574	3173	3183	3190	rBV2	17725	31061	3.94%	0.441%
90	11.697	3215	3221	3230	rVB5	22141	34472	4.37%	0.490%
91	11.812	3247	3257	3270	rVB	444757	696146	88.23%	9.888%
92	11.941	3293	3297	3302	rBV2	8071	10693	1.36%	0.152%
93	12.195	3361	3376	3389	rVB	403464	653341	82.81%	9.280%
94	12.327	3412	3417	3427	rVB6	10570	15206	1.93%	0.216%
95	12.668	3517	3523	3531	rVB3	15442	21070	2.67%	0.299%
96	13.587	3803	3809	3815	rBV3	12307	17131	2.17%	0.243%
97	14.086	3957	3964	3973	rBV	34827	49395	6.26%	0.702%
98	14.452	4073	4078	4084	rBV7	3316	4566	0.58%	0.065%
99	15.221	4306	4317	4329	rVB3	7223	15928	2.02%	0.226%
100	16.192	4612	4619	4635	rBV10	7777	14238	1.80%	0.202%

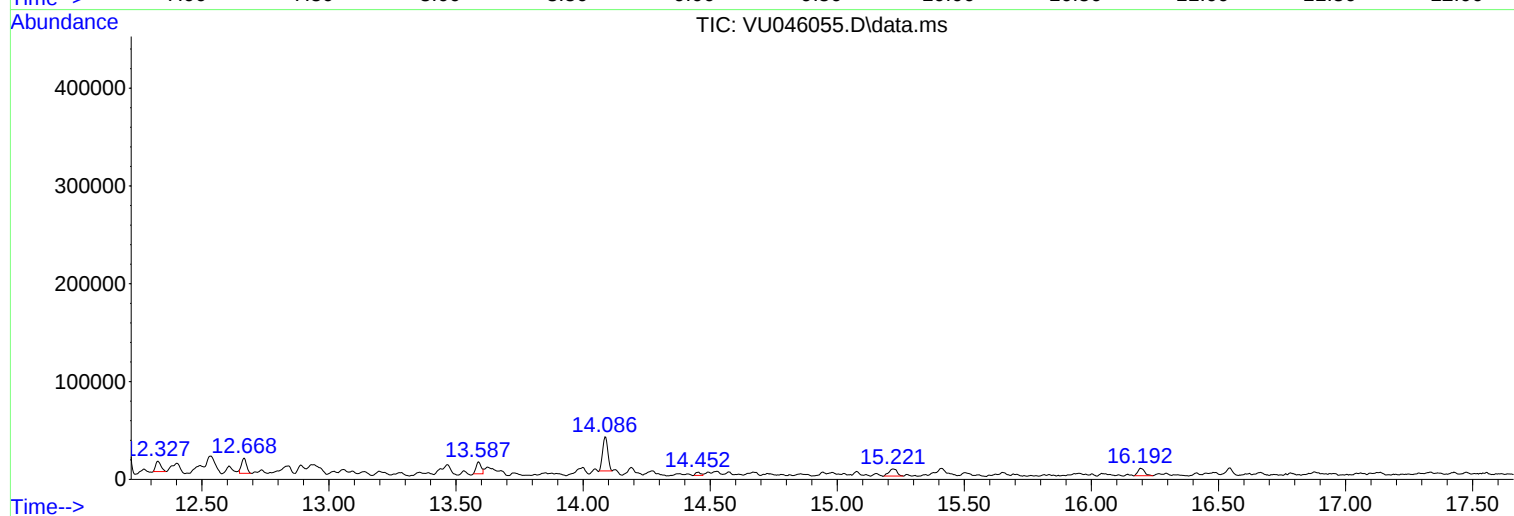
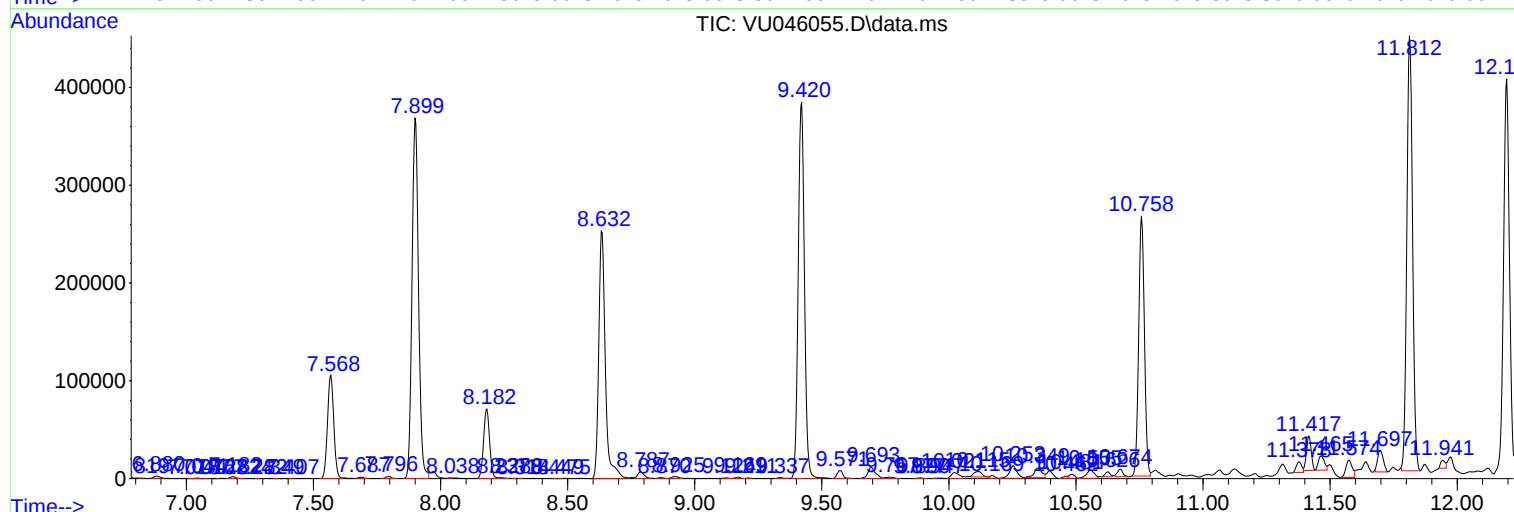
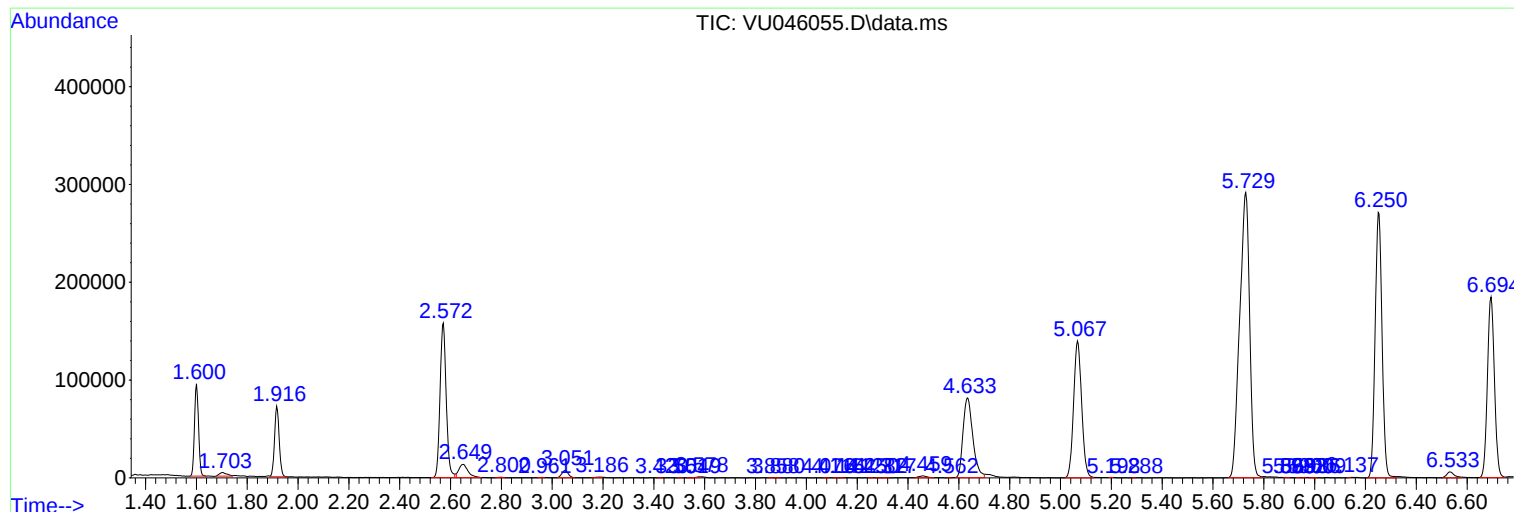
Sum of corrected areas: 7040139

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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



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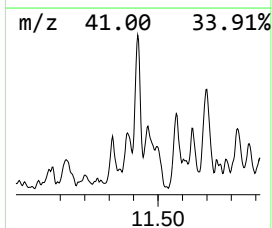
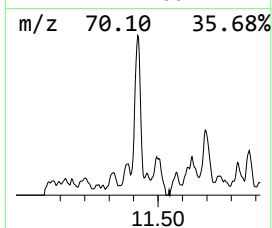
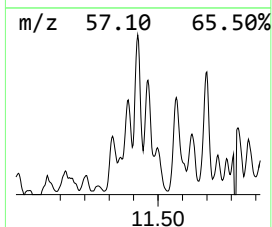
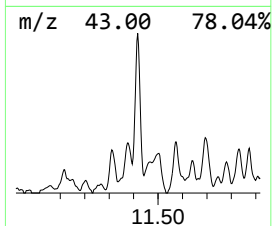
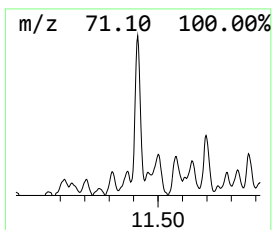
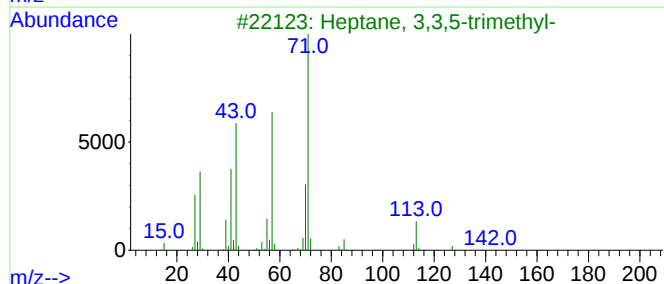
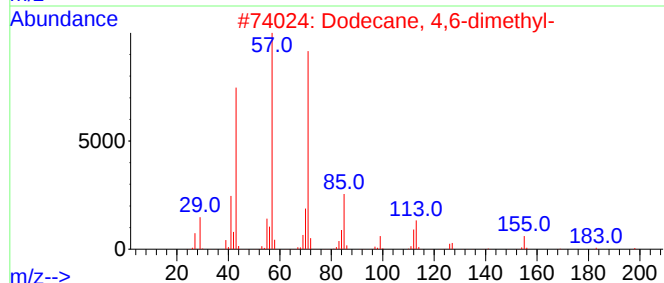
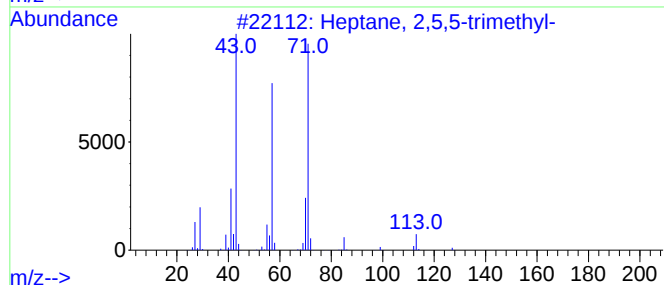
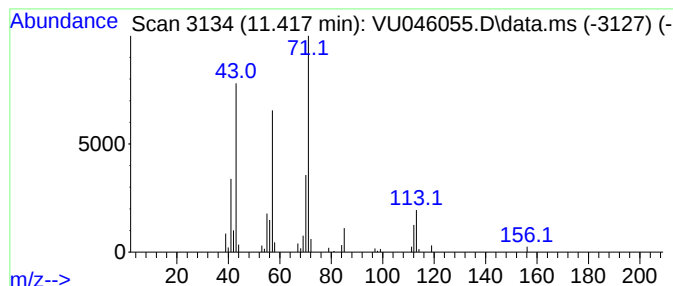
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.417	3.29 ug/L	45874	1,4-Dichlorobenzene-d4	11.812

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptane, 2,5,5-trimethyl-	142	C10H22	001189-99-7	78
2		Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	72
3		Heptane, 3,3,5-trimethyl-	142	C10H22	007154-80-5	72
4		Decane, 4-methyl-	156	C11H24	002847-72-5	72
5		Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	64



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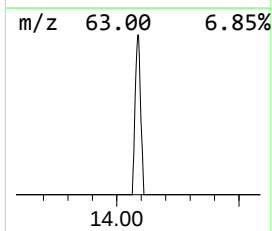
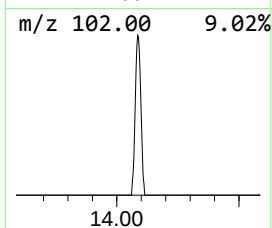
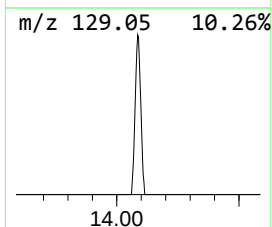
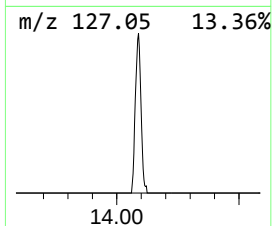
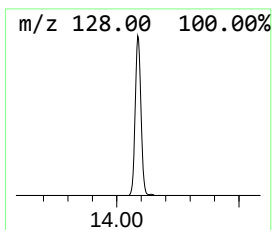
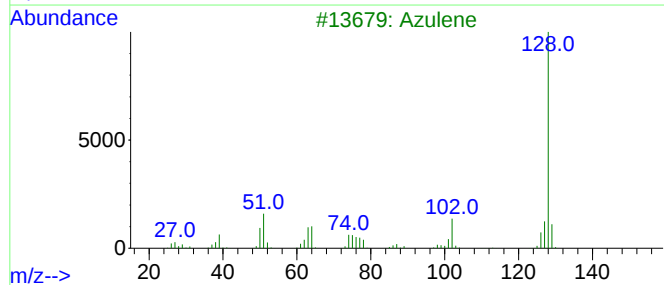
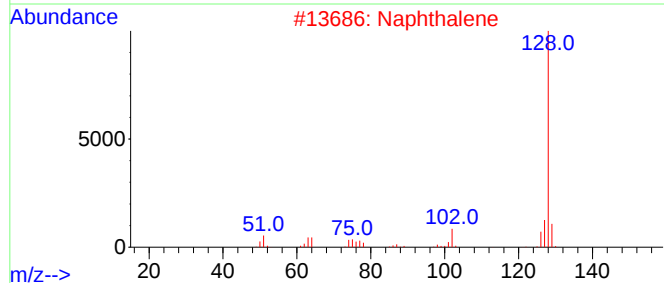
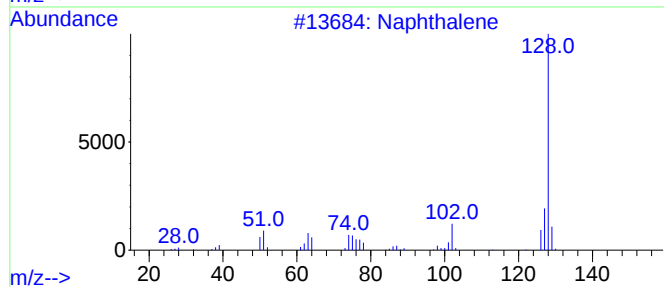
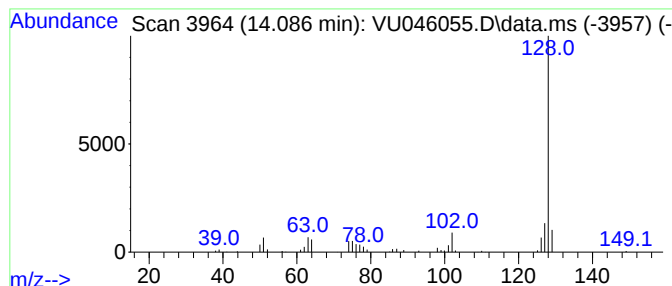
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Quant Title : VOC Analysis

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

Peak Number 3 Azulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.086	3.55 ug/L	49395	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	97
2			Naphthalene	128	C10H8	000091-20-3	95
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\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	11.417	3.3	ug/L	45874	3	11.812	696146	50.0
Azulene	14.086	3.5	ug/L	49395	3	11.812	696146	50.0