

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011422\
 Data File : VV024366.D
 Acq On : 14 Jan 2022 17:14
 Operator : SY/MD
 Sample : N1114-09ME
 Misc : 6.19g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BGLQ1ME

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_V\Method\SFAMVLM123121WMA.M
 Title : VOC Analysis

Signal : TIC: VV024366.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.304	76	82	102	rVB	150407	180008	10.37%	1.190%
2	1.564	157	163	178	rBV	113430	136374	7.85%	0.902%
3	2.095	317	328	354	rBV3	396998	645271	37.17%	4.268%
4	2.503	447	455	466	rVB3	3524	5563	0.32%	0.037%
5	2.883	571	573	576	rBV2	350	153	0.01%	0.001%
6	2.960	593	597	600	rBV2	258	202	0.01%	0.001%
7	3.185	651	667	687	rBV	49180	104323	6.01%	0.690%
8	3.326	708	711	712	rBV	298	150	0.01%	0.001%
9	3.420	735	740	743	rBV2	456	401	0.02%	0.003%
10	3.606	796	798	801	rBV2	188	146	0.01%	0.001%
11	3.841	868	871	872	rBV	241	114	0.01%	0.001%
12	3.886	875	885	912	rBV	91457	293989	16.93%	1.944%
13	4.346	1013	1028	1063	rVB2	261835	706557	40.69%	4.673%
14	4.728	1144	1147	1149	rBV	468	263	0.02%	0.002%
15	4.757	1154	1156	1158	rVB	309	132	0.01%	0.001%
16	4.770	1158	1160	1164	rBV2	390	196	0.01%	0.001%
17	4.937	1209	1212	1214	rBV	192	161	0.01%	0.001%
18	5.040	1227	1244	1288	rBV2	601341	1508451	86.88%	9.976%
19	5.612	1410	1422	1456	rBV	508234	1016909	58.57%	6.725%
20	5.911	1501	1515	1534	rBV2	284224	584703	33.68%	3.867%
21	6.066	1550	1563	1594	rVB	331506	671022	38.65%	4.438%
22	6.268	1624	1626	1629	rVB	432	183	0.01%	0.001%
23	6.288	1629	1632	1634	rBV	376	272	0.02%	0.002%
24	6.320	1638	1642	1644	rBV	339	172	0.01%	0.001%
25	6.426	1671	1675	1678	rVB3	358	297	0.02%	0.002%
26	6.516	1692	1703	1711	rBV6	4328	8378	0.48%	0.055%
27	6.571	1717	1720	1723	rVB2	527	361	0.02%	0.002%
28	6.596	1723	1728	1729	rBV2	303	303	0.02%	0.002%
29	6.638	1733	1741	1745	rBV6	2514	3883	0.22%	0.026%
30	6.725	1766	1768	1769	rBV	442	196	0.01%	0.001%
31	6.773	1780	1783	1785	rBV	329	189	0.01%	0.001%
32	6.982	1837	1848	1873	rBV	192871	358491	20.65%	2.371%
33	7.313	1938	1951	1967	rBV	716576	1244176	71.66%	8.228%
34	7.580	2032	2034	2036	rBV2	332	137	0.01%	0.001%
35	7.619	2036	2046	2069	rBV	128644	244397	14.08%	1.616%
36	7.847	2115	2117	2119	rVB2	432	161	0.01%	0.001%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.M
 Title : VOC Analysis

37	7.927	2140	2142	2143	rBV2	263	106	0.01%	0.001%
38	7.973	2143	2156	2176	rBV	1051577	1736230	100.00%	11.483%
39	8.111	2184	2199	2233	rBV4	225866	740581	42.65%	4.898%
40	8.603	2350	2352	2354	rBV2	282	177	0.01%	0.001%
41	8.622	2355	2358	2359	rVV2	257	142	0.01%	0.001%
42	8.670	2370	2373	2378	rBV2	604	537	0.03%	0.004%
43	8.789	2406	2410	2415	rVB4	479	357	0.02%	0.002%
44	8.853	2418	2430	2456	rBV	708512	1222223	70.40%	8.083%
45	9.017	2475	2481	2493	rBV3	5133	8377	0.48%	0.055%
46	9.143	2511	2520	2535	rBV2	15647	29407	1.69%	0.194%
47	9.336	2577	2580	2582	rBV	193	127	0.01%	0.001%
48	9.448	2613	2615	2618	rBV	290	137	0.01%	0.001%
49	9.471	2620	2622	2624	rBV	304	139	0.01%	0.001%
50	9.554	2638	2648	2661	rBV4	3482	6346	0.37%	0.042%
51	9.609	2662	2665	2667	rBV2	431	225	0.01%	0.001%
52	9.677	2684	2686	2687	rBV	399	144	0.01%	0.001%
53	9.706	2691	2695	2696	rBV2	771	576	0.03%	0.004%
54	9.741	2704	2706	2709	rBV2	191	123	0.01%	0.001%
55	9.773	2712	2716	2717	rBV2	273	185	0.01%	0.001%
56	9.841	2735	2737	2739	rBV	372	230	0.01%	0.002%
57	9.937	2759	2767	2775	rBV4	2755	4102	0.24%	0.027%
58	10.017	2788	2792	2799	rVB4	1244	1391	0.08%	0.009%
59	10.069	2802	2808	2809	rBV3	728	724	0.04%	0.005%
60	10.220	2841	2855	2874	rVV	429322	731148	42.11%	4.835%
61	10.416	2913	2916	2918	rVB2	287	158	0.01%	0.001%
62	10.455	2922	2928	2932	rBV5	2612	3375	0.19%	0.022%
63	10.542	2949	2955	2957	rBV3	1602	1477	0.09%	0.010%
64	10.577	2961	2966	2983	rVB2	15462	23355	1.35%	0.154%
65	10.706	3004	3006	3009	rBV3	376	171	0.01%	0.001%
66	10.741	3012	3017	3021	rBV2	1770	1601	0.09%	0.011%
67	10.763	3022	3024	3026	rBV2	787	366	0.02%	0.002%
68	10.876	3055	3059	3065	rBV4	3306	3690	0.21%	0.024%
69	11.033	3099	3108	3116	rBV9	2248	3807	0.22%	0.025%
70	11.249	3164	3175	3197	rBV	805956	1245827	71.75%	8.239%
71	11.503	3252	3254	3255	rBV	462	169	0.01%	0.001%
72	11.625	3280	3292	3311	rBV	787290	1232453	70.98%	8.151%
73	11.789	3336	3343	3352	rVB3	21063	29583	1.70%	0.196%
74	11.914	3376	3382	3383	rBV4	1414	1104	0.06%	0.007%
75	12.223	3474	3478	3481	rBV	332	344	0.02%	0.002%
76	12.262	3488	3490	3497	rVB5	1204	866	0.05%	0.006%

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 BGLQ1ME

Integration Parameters: LSCINT.P

Integrator: RTE

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77	12.371	3515	3524	3529	rBV6	2580	4034	0.23%	0.027%
78	12.580	3587	3589	3590	rBV	1111	513	0.03%	0.003%
79	12.664	3613	3615	3618	rVB2	429	169	0.01%	0.001%
80	12.747	3640	3641	3645	rBV2	337	234	0.01%	0.002%
81	12.770	3645	3648	3649	rBV	445	218	0.01%	0.001%
82	12.885	3677	3684	3693	rBV3	9594	13782	0.79%	0.091%
83	12.956	3702	3706	3708	rBV3	453	334	0.02%	0.002%
84	13.194	3778	3780	3784	rBV3	435	358	0.02%	0.002%
85	13.217	3784	3787	3790	rBV2	599	382	0.02%	0.003%
86	13.316	3816	3818	3819	rBV	360	127	0.01%	0.001%
87	13.355	3829	3830	3834	rBV3	490	212	0.01%	0.001%
88	13.448	3858	3859	3860	rBV	566	178	0.01%	0.001%
89	13.503	3866	3876	3897	rVB	117198	192428	11.08%	1.273%
90	13.628	3907	3915	3926	rBV7	3353	6610	0.38%	0.044%
91	13.824	3974	3976	3982	rVB4	880	909	0.05%	0.006%
92	13.850	3982	3984	3985	rBV	811	348	0.02%	0.002%
93	13.963	4015	4019	4021	rBV4	644	537	0.03%	0.004%
94	14.040	4042	4043	4048	rVB5	911	436	0.03%	0.003%
95	14.361	4141	4143	4145	rBV2	888	477	0.03%	0.003%
96	14.506	4181	4188	4189	rBV4	1073	1251	0.07%	0.008%
97	14.631	4218	4227	4241	rBV	53424	85417	4.92%	0.565%
98	14.818	4277	4285	4303	rVB5	19639	38623	2.22%	0.255%
99	15.085	4366	4368	4369	rBV	827	312	0.02%	0.002%
100	15.667	4542	4549	4559	rVB4	15129	23838	1.37%	0.158%

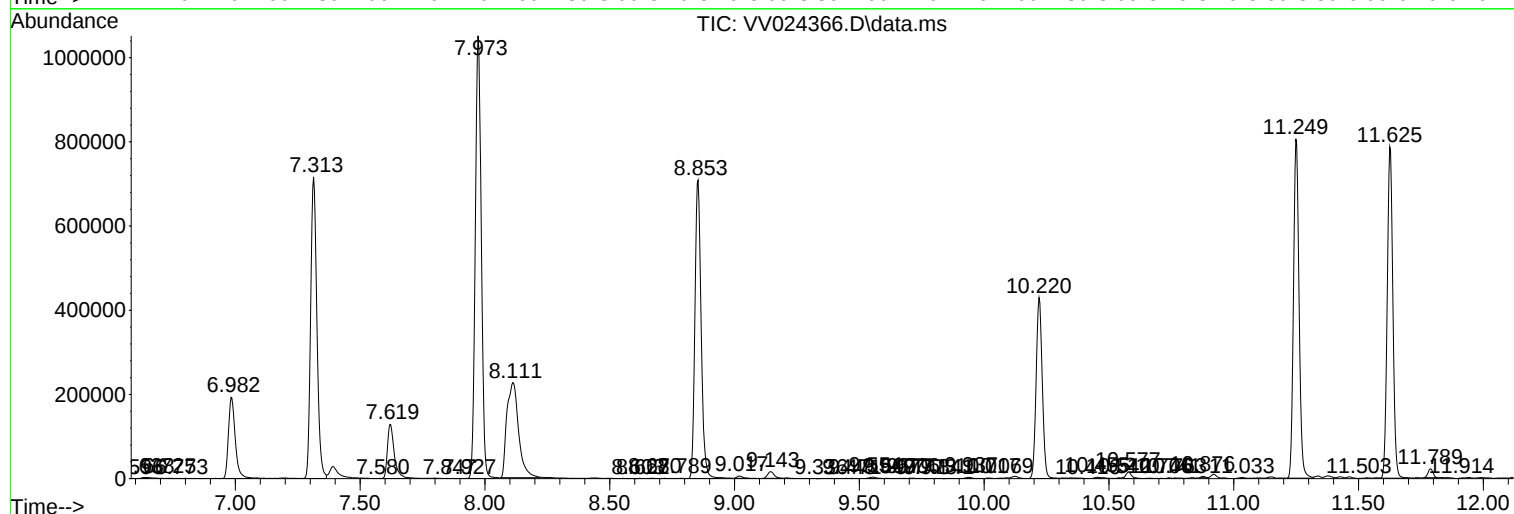
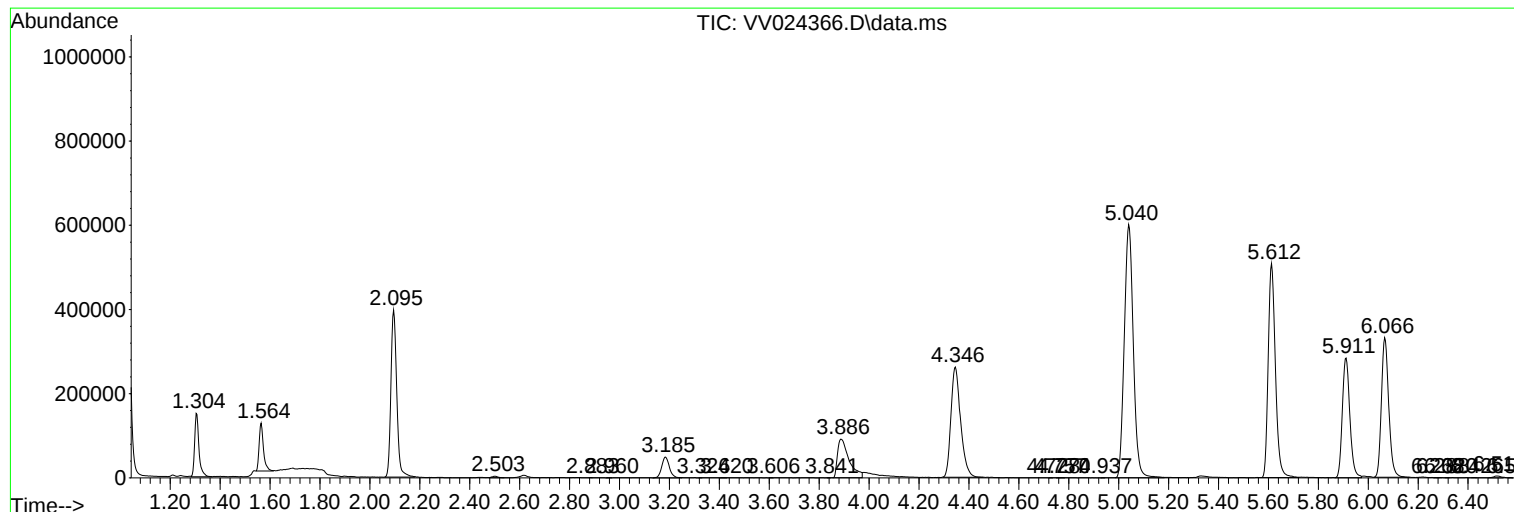
Sum of corrected areas: 15120491

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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGLQ1ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.M
Quant Title : VOC Analysis

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



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Instrument :
MSVOA_V
ClientSampleId :
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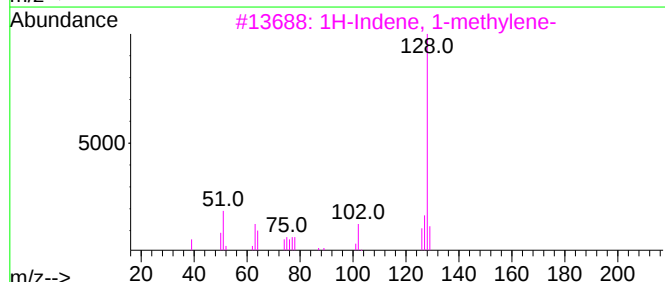
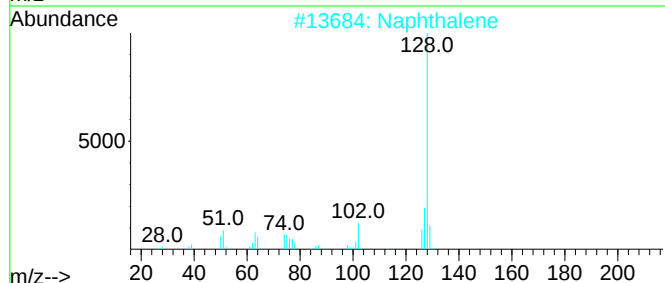
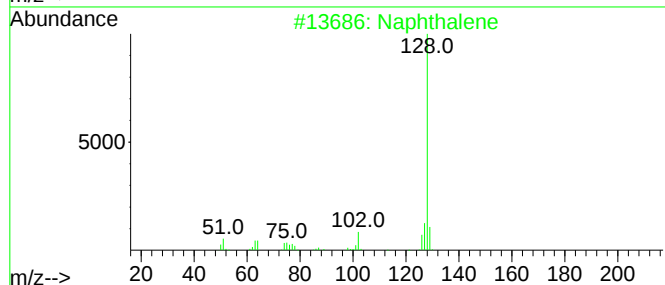
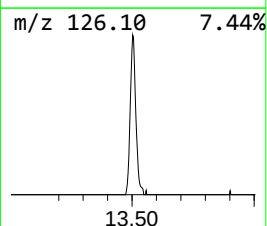
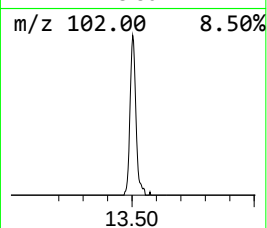
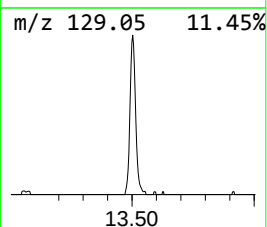
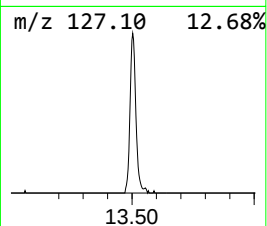
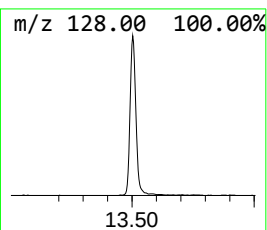
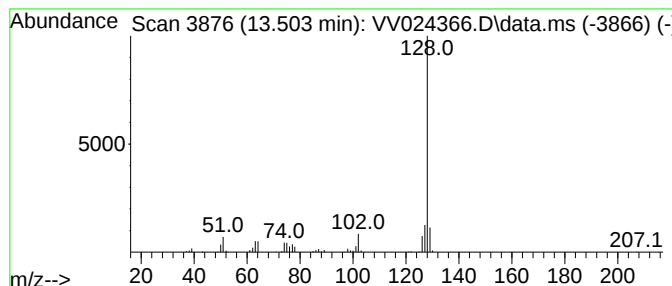
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Azulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.503	7.72 ug/L	192428	1,4-Dichlorobenzene-d4	11.249

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			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	91
4			Azulene	128	C10H8	000275-51-4	91
5			Azulene	128	C10H8	000275-51-4	90



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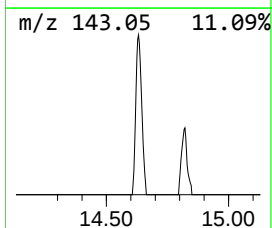
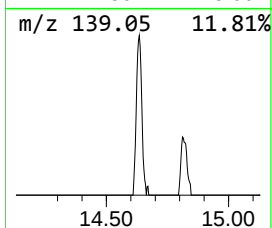
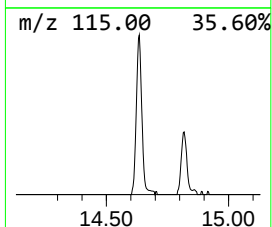
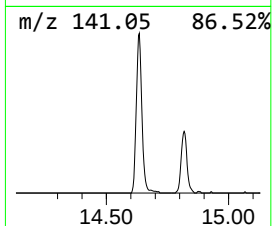
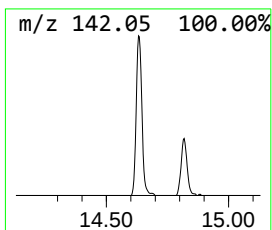
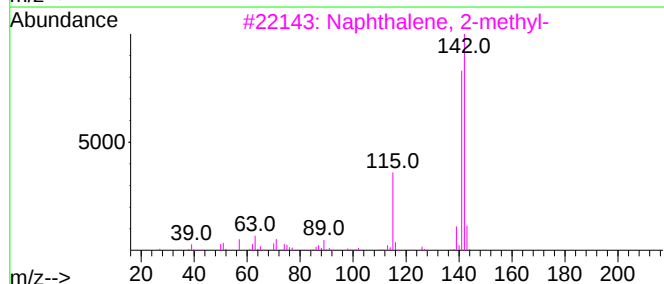
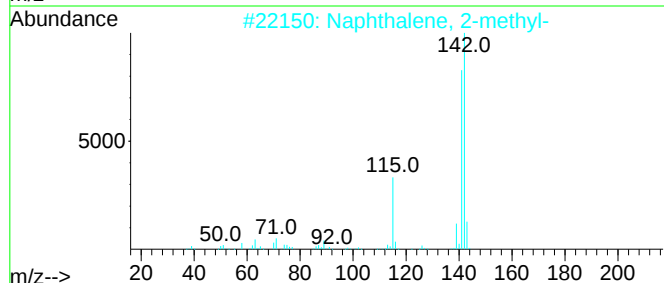
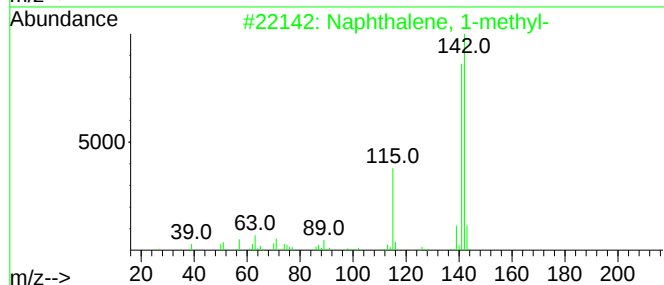
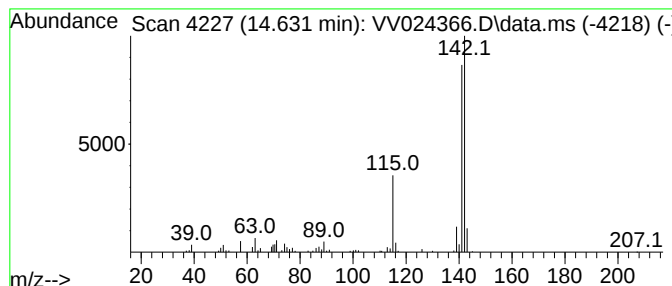
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Naphthalene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.631	3.43 ug/L	85417	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
4			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94
5			Benzocycloheptatriene	142	C11H10	000264-09-5	94



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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
Azulene	13.503	7.7	ug/L	192428	3	11.249	1245830	50.0
Naphthalene, 1-...	14.631	3.4	ug/L	85417	3	11.249	1245830	50.0