

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
 Data File : VU046144.D
 Acq On : 07 Dec 2021 16:35
 Operator : SY/MD
 Sample : M4960-11DL 40X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGKS4DL

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: VU046144.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	74	81	101	rVB	115770	128541	14.82%	1.570%
2	1.919	171	180	192	rBV	80923	103882	11.97%	1.269%
3	2.379	313	323	336	rVB	14704	21882	2.52%	0.267%
4	2.511	361	364	369	rVB2	361	286	0.03%	0.003%
5	2.572	371	383	402	rBV	188865	313357	36.12%	3.827%
6	2.806	450	456	459	rBV2	279	255	0.03%	0.003%
7	2.951	498	501	505	rVB	332	245	0.03%	0.003%
8	3.051	522	532	543	rBV3	2783	5267	0.61%	0.064%
9	3.186	564	574	588	rVB	1822	3549	0.41%	0.043%
10	3.359	624	628	631	rVV	265	241	0.03%	0.003%
11	3.446	649	655	657	rBV	145	200	0.02%	0.002%
12	3.880	779	790	794	rVV3	867	1702	0.20%	0.021%
13	4.642	1009	1027	1068	rBV3	73263	276789	31.90%	3.381%
14	5.067	1143	1159	1183	rBV	141521	326598	37.64%	3.989%
15	5.273	1219	1223	1227	rVB	245	198	0.02%	0.002%
16	5.301	1228	1232	1234	rBV	280	209	0.02%	0.003%
17	5.314	1234	1236	1240	rVB	300	206	0.02%	0.003%
18	5.594	1318	1323	1327	rBB	150	205	0.02%	0.003%
19	5.729	1343	1365	1377	rBV2	319273	867596	100.00%	10.597%
20	5.935	1426	1429	1439	rBV2	158	269	0.03%	0.003%
21	6.054	1464	1466	1470	rVB2	344	237	0.03%	0.003%
22	6.157	1492	1498	1500	rBV2	850	785	0.09%	0.010%
23	6.253	1513	1528	1548	rBV	297301	565253	65.15%	6.904%
24	6.533	1603	1615	1627	rBV6	3214	6703	0.77%	0.082%
25	6.694	1651	1665	1681	rBV	189911	369082	42.54%	4.508%
26	6.935	1738	1740	1744	rVB	286	196	0.02%	0.002%
27	7.218	1825	1828	1832	rBV	254	207	0.02%	0.003%
28	7.568	1923	1937	1950	rBV	111981	193926	22.35%	2.369%
29	7.797	1999	2008	2015	rBV3	1447	1934	0.22%	0.024%
30	7.899	2025	2040	2053	rBV	415826	721900	83.21%	8.817%
31	7.970	2053	2062	2092	rVB	106757	190205	21.92%	2.323%
32	8.182	2115	2128	2141	rBV	76170	127564	14.70%	1.558%
33	8.276	2155	2157	2161	rVB	375	275	0.03%	0.003%
34	8.472	2214	2218	2222	rVB2	272	301	0.03%	0.004%
35	8.552	2239	2243	2246	rBV	248	191	0.02%	0.002%
36	8.636	2254	2269	2301	rBV	253944	446432	51.46%	5.453%

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 Title : VOC Analysis

37	8.915	2349	2356	2361	rBV	667	908	0.10%	0.011%
38	9.420	2498	2513	2538	rBV2	426751	810934	93.47%	9.905%
39	9.571	2549	2560	2581	rVB	42948	69232	7.98%	0.846%
40	9.694	2585	2598	2616	rVV	105558	172948	19.93%	2.112%
41	9.780	2617	2625	2636	rVB2	1251	1945	0.22%	0.024%
42	9.922	2664	2669	2673	rVB2	404	467	0.05%	0.006%
43	10.102	2714	2725	2740	rBV2	44392	76764	8.85%	0.938%
44	10.240	2761	2768	2775	rVB2	968	1444	0.17%	0.018%
45	10.485	2835	2844	2855	rBV	5407	8472	0.98%	0.103%
46	10.568	2859	2870	2885	rVB	72406	118997	13.72%	1.453%
47	10.671	2893	2902	2911	rBV4	2868	4792	0.55%	0.059%
48	10.758	2917	2929	2946	rVB	276201	442976	51.06%	5.411%
49	10.870	2958	2964	2967	rBV2	551	618	0.07%	0.008%
50	10.906	2967	2975	2987	rVB2	2572	5027	0.58%	0.061%
51	10.999	2987	3004	3023	rBV	12575	26158	3.01%	0.319%
52	11.089	3023	3032	3039	rBV	6864	10473	1.21%	0.128%
53	11.295	3086	3096	3105	rBV3	6068	9081	1.05%	0.111%
54	11.378	3117	3122	3126	rBV	267	267	0.03%	0.003%
55	11.417	3129	3134	3139	rBV4	501	544	0.06%	0.007%
56	11.468	3139	3150	3165	rVB	28265	43986	5.07%	0.537%
57	11.539	3165	3172	3177	rBV4	947	1308	0.15%	0.016%
58	11.571	3177	3182	3184	rBV3	1332	1134	0.13%	0.014%
59	11.645	3200	3205	3210	rBV2	311	313	0.04%	0.004%
60	11.697	3214	3221	3228	rBV4	1528	2243	0.26%	0.027%
61	11.735	3228	3233	3242	rVB5	923	1244	0.14%	0.015%
62	11.812	3243	3257	3274	rBV	499894	786658	90.67%	9.608%
63	11.896	3275	3283	3292	rVB2	9021	12028	1.39%	0.147%
64	11.941	3292	3297	3301	rBV5	628	774	0.09%	0.009%
65	12.063	3329	3335	3337	rBV4	1188	1238	0.14%	0.015%
66	12.092	3338	3344	3359	rVV3	5577	9456	1.09%	0.115%
67	12.195	3359	3376	3391	rVV	430767	706428	81.42%	8.628%
68	12.266	3396	3398	3401	rVB3	411	206	0.02%	0.003%
69	12.324	3406	3416	3425	rVB8	3099	5827	0.67%	0.071%
70	12.401	3427	3440	3445	rBV7	703	1665	0.19%	0.020%
71	12.465	3453	3460	3465	rBV4	1157	1796	0.21%	0.022%
72	12.571	3485	3493	3504	rBV4	1695	2605	0.30%	0.032%
73	12.681	3523	3527	3530	rBV2	591	637	0.07%	0.008%
74	12.774	3551	3556	3564	rVB3	1040	1128	0.13%	0.014%
75	12.877	3582	3588	3592	rBV4	566	647	0.07%	0.008%
76	12.954	3603	3612	3626	rBV7	3871	7413	0.85%	0.091%

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77	13.031	3629	3636	3644	rVB5	1802	2511	0.29%	0.031%
78	13.140	3668	3670	3673	rBV2	507	326	0.04%	0.004%
79	13.269	3700	3710	3723	rBV7	2772	5333	0.61%	0.065%
80	13.346	3731	3734	3736	rBV3	404	223	0.03%	0.003%
81	13.436	3755	3762	3763	rBV4	1213	1087	0.13%	0.013%
82	13.517	3782	3787	3793	rVB2	940	965	0.11%	0.012%
83	13.626	3816	3821	3824	rBV4	816	766	0.09%	0.009%
84	13.738	3849	3856	3864	rVV4	2329	3186	0.37%	0.039%
85	13.835	3882	3886	3888	rBV2	784	628	0.07%	0.008%
86	13.870	3893	3897	3903	rVB2	1185	1300	0.15%	0.016%
87	13.938	3915	3918	3922	rVB2	363	258	0.03%	0.003%
88	14.086	3952	3964	3978	rBV	69292	111805	12.89%	1.366%
89	14.160	3984	3987	3990	rVB2	476	352	0.04%	0.004%
90	14.298	4027	4030	4034	rVB2	599	333	0.04%	0.004%
91	14.423	4064	4069	4073	rBV4	569	594	0.07%	0.007%
92	14.484	4086	4088	4094	rVB3	347	260	0.03%	0.003%
93	14.574	4112	4116	4124	rVB4	1359	1717	0.20%	0.021%
94	14.861	4203	4205	4211	rVB3	599	526	0.06%	0.006%
95	14.896	4212	4216	4220	rBV3	356	303	0.03%	0.004%
96	14.960	4229	4236	4238	rBV2	293	407	0.05%	0.005%
97	15.224	4308	4318	4334	rVB	11076	17041	1.96%	0.208%
98	15.407	4366	4375	4387	rBV2	5272	8451	0.97%	0.103%
99	15.951	4542	4544	4554	rVB3	1059	1093	0.13%	0.013%
100	16.179	4613	4615	4618	rBV2	407	314	0.04%	0.004%

Sum of corrected areas: 8187228

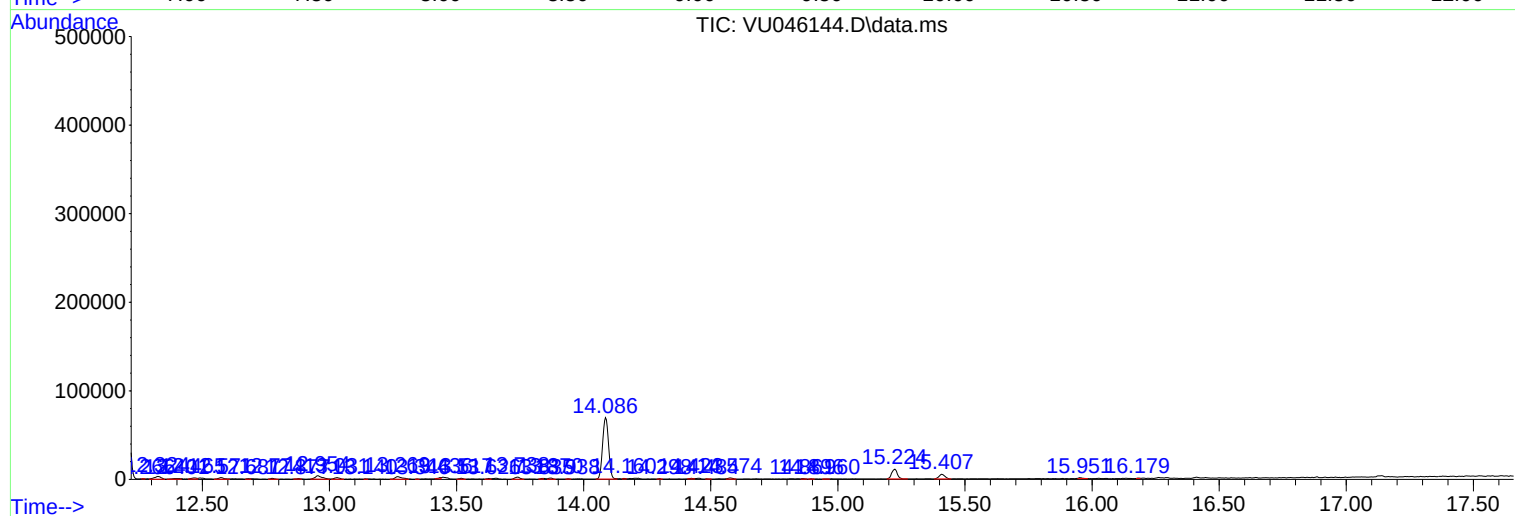
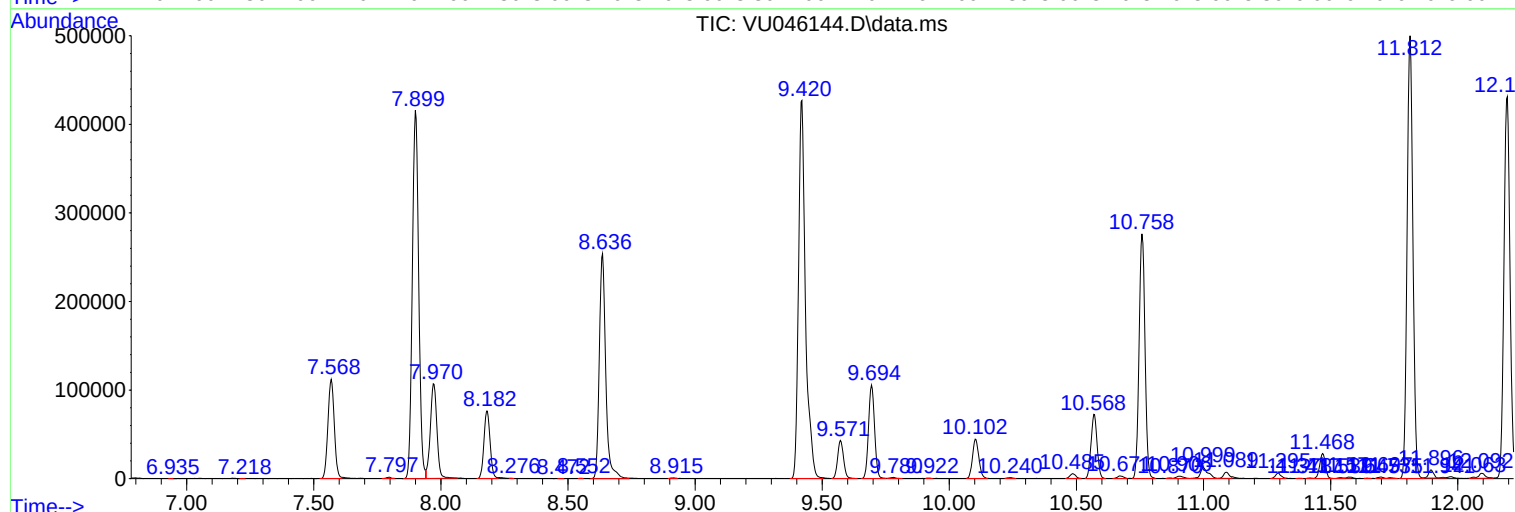
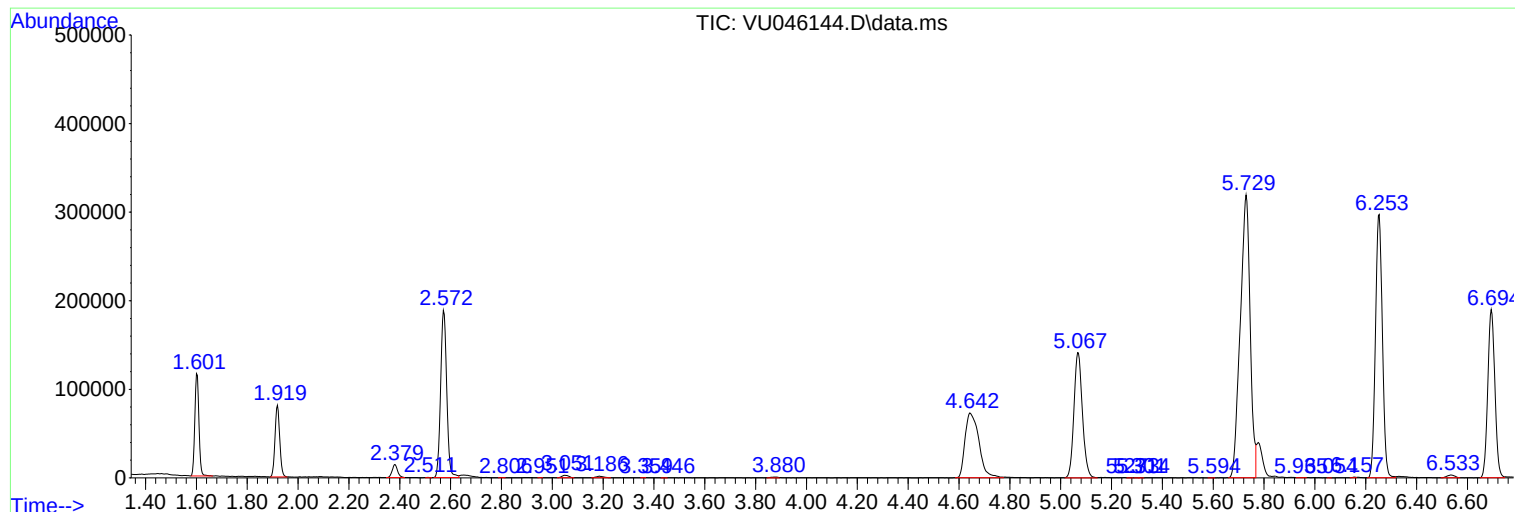
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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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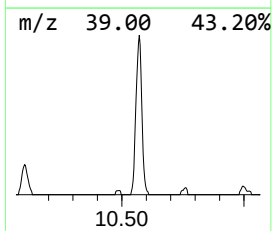
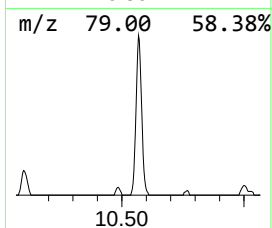
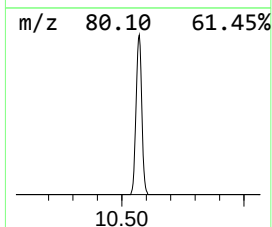
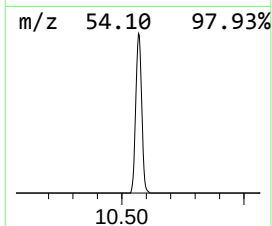
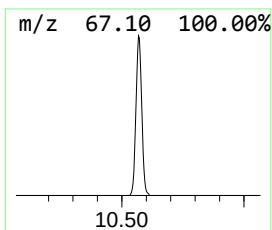
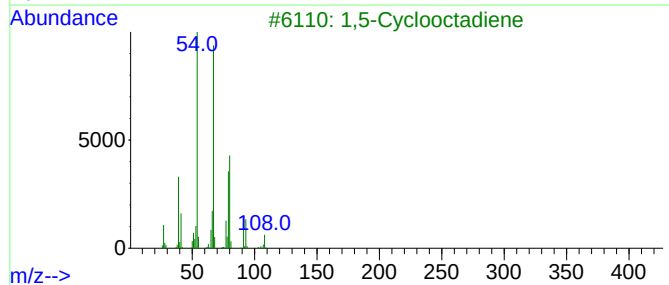
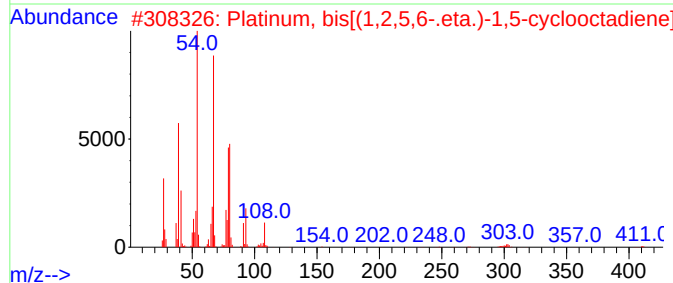
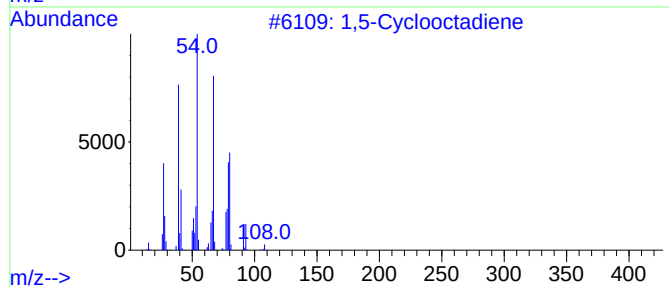
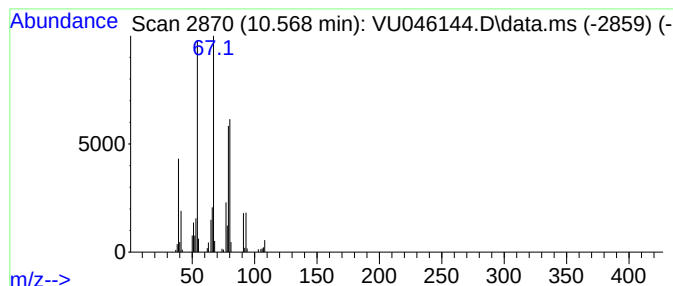
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 1,5-Cyclooctadiene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.568	7.34 ug/L	118997	Chlorobenzene-d5	9.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,5-Cyclooctadiene			108	C8H12	000111-78-4	94
2	Platinum, bis[(1,2,5,6-.eta.)-1,...			411	C16H24Pt	012130-66-4	87
3	1,5-Cyclooctadiene			108	C8H12	000111-78-4	80
4	1,5-Cyclooctadiene			108	C8H12	000111-78-4	78
5	1,5-Cyclooctadiene			108	C8H12	000111-78-4	74



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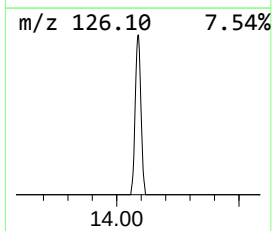
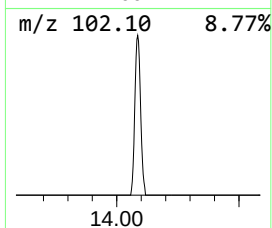
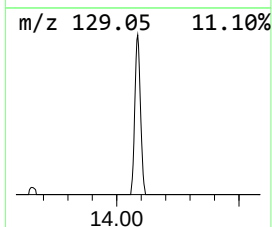
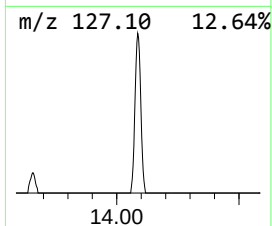
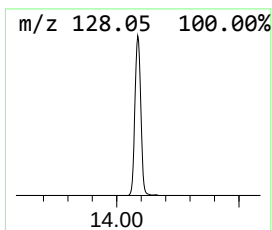
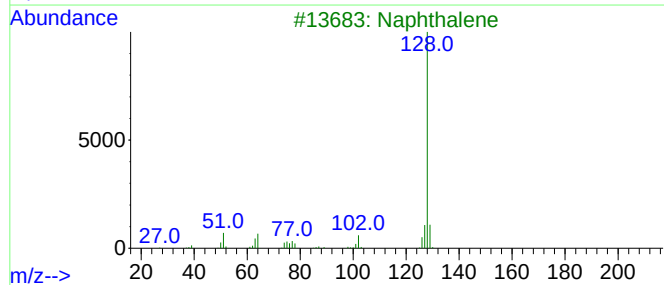
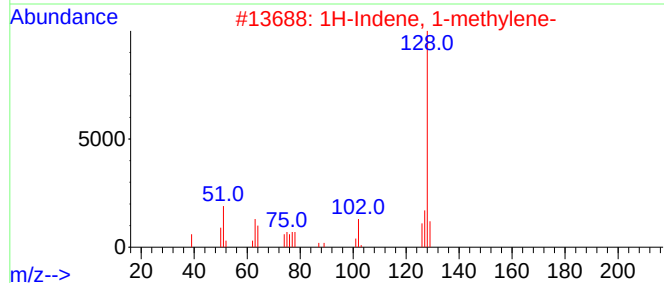
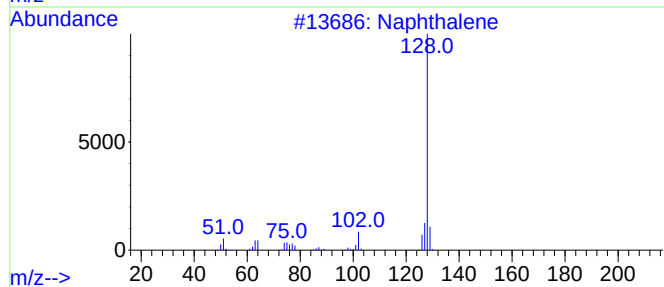
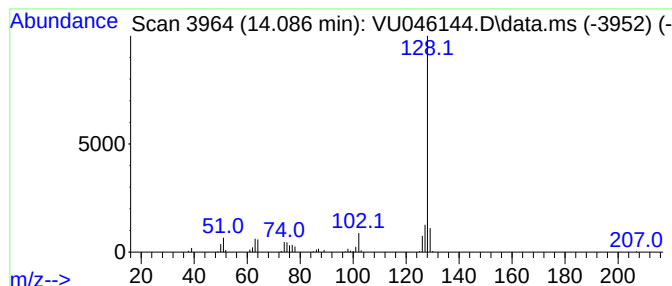
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Azulene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.086	7.11 ug/L	111805	1,4-Dichlorobenzene-d4	11.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	95
3			Naphthalene	128	C10H8	000091-20-3	94
4			Azulene	128	C10H8	000275-51-4	91
5			Azulene	128	C10H8	000275-51-4	91



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,5-Cyclooctadiene	10.568	7.3	ug/L	118997	2	9.420	810934	50.0
Azulene	14.086	7.1	ug/L	111805	3	11.813	786658	50.0