

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU032422\
 Data File : VU047652.D
 Acq On : 24 Mar 2022 23:01
 Operator : SY/MD
 Sample : N2081-11
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW5X8

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\SFAMULM032422WMA.M
 Title : VOC Analysis

Signal : TIC: VU047652.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.604	74	82	99	rVB	83686	98606	2.43%	0.686%
2	1.919	172	180	197	rBV	63112	85147	2.10%	0.593%
3	2.575	370	384	404	rBV2	166132	319493	7.88%	2.224%
4	2.784	444	449	451	rBV2	760	647	0.02%	0.005%
5	2.803	451	455	464	rVB3	1054	1570	0.04%	0.011%
6	2.884	476	480	484	rBV3	332	370	0.01%	0.003%
7	3.054	527	533	534	rBV3	310	300	0.01%	0.002%
8	3.096	543	546	550	rVB2	377	289	0.01%	0.002%
9	3.195	574	577	583	rVB3	635	578	0.01%	0.004%
10	3.228	583	587	590	rBV4	333	323	0.01%	0.002%
11	3.257	593	596	603	rVB3	303	318	0.01%	0.002%
12	3.359	616	628	645	rVB	21392	42720	1.05%	0.297%
13	3.726	734	742	745	rBV3	333	418	0.01%	0.003%
14	3.874	769	788	810	rBV	319767	759810	18.74%	5.289%
15	4.070	845	849	852	rVB2	315	297	0.01%	0.002%
16	4.118	859	864	866	rBV2	486	440	0.01%	0.003%
17	4.221	893	896	904	rVB3	395	325	0.01%	0.002%
18	4.285	910	916	920	rBV3	310	441	0.01%	0.003%
19	4.417	954	957	962	rBV3	349	316	0.01%	0.002%
20	4.488	974	979	982	rBV2	318	299	0.01%	0.002%
21	4.671	1012	1036	1069	rBV	1128701	2696350	66.49%	18.771%
22	5.067	1143	1159	1180	rBV	115618	260166	6.42%	1.811%
23	5.163	1187	1189	1193	rVB3	499	257	0.01%	0.002%
24	5.224	1206	1208	1213	rVB3	362	258	0.01%	0.002%
25	5.321	1218	1238	1276	rVV	1807152	4055012	100.00%	28.229%
26	5.729	1342	1365	1396	rVV2	235306	649454	16.02%	4.521%
27	5.996	1442	1448	1449	rBV2	227	259	0.01%	0.002%
28	6.160	1496	1499	1503	rVB2	303	252	0.01%	0.002%
29	6.186	1503	1507	1510	rBV2	270	266	0.01%	0.002%
30	6.250	1512	1527	1553	rBV	332863	626304	15.45%	4.360%
31	6.427	1579	1582	1585	rBV2	451	301	0.01%	0.002%
32	6.546	1607	1619	1634	rBV	44986	83007	2.05%	0.578%
33	6.694	1651	1665	1684	rBV	140981	277875	6.85%	1.934%
34	6.916	1729	1734	1738	rVB3	461	380	0.01%	0.003%
35	7.102	1789	1792	1796	rVB2	304	258	0.01%	0.002%
36	7.128	1797	1800	1806	rVB3	318	309	0.01%	0.002%

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 Title : VOC Analysis

37	7.305	1852	1855	1861	rBV3	328	302	0.01%	0.002%
38	7.485	1908	1911	1915	rVB2	382	312	0.01%	0.002%
39	7.568	1923	1937	1953	rBV	81277	146217	3.61%	1.018%
40	7.797	2002	2008	2009	rBV3	2349	2136	0.05%	0.015%
41	7.899	2024	2040	2055	rBV	286591	505002	12.45%	3.516%
42	8.060	2085	2090	2094	rBV3	418	386	0.01%	0.003%
43	8.179	2112	2127	2149	rBV3	64391	127676	3.15%	0.889%
44	8.404	2189	2197	2204	rVB5	2822	4640	0.11%	0.032%
45	8.472	2211	2218	2228	rBV2	3388	5217	0.13%	0.036%
46	8.555	2232	2244	2258	rBV	116055	197745	4.88%	1.377%
47	8.639	2258	2270	2301	rVV	197327	382957	9.44%	2.666%
48	8.954	2365	2368	2373	rVV3	353	314	0.01%	0.002%
49	8.993	2375	2380	2385	rVB3	313	323	0.01%	0.002%
50	9.018	2385	2388	2391	rBV2	339	273	0.01%	0.002%
51	9.311	2474	2479	2481	rBV2	242	252	0.01%	0.002%
52	9.417	2498	2512	2534	rBV	477265	806996	19.90%	5.618%
53	9.575	2553	2561	2574	rVB2	5105	7320	0.18%	0.051%
54	9.694	2587	2598	2614	rBV	12658	21122	0.52%	0.147%
55	9.851	2642	2647	2649	rBV2	291	315	0.01%	0.002%
56	10.028	2698	2702	2708	rVB3	481	556	0.01%	0.004%
57	10.102	2716	2725	2738	rVB4	6949	11840	0.29%	0.082%
58	10.449	2830	2833	2838	rVB3	440	464	0.01%	0.003%
59	10.481	2838	2843	2852	rBV3	1728	2762	0.07%	0.019%
60	10.604	2877	2881	2884	rBV2	314	302	0.01%	0.002%
61	10.671	2895	2902	2913	rVB4	1210	1937	0.05%	0.013%
62	10.758	2917	2929	2946	rVV	217690	352737	8.70%	2.456%
63	10.896	2960	2972	2988	rVB4	9023	16704	0.41%	0.116%
64	10.999	2994	3004	3023	rVV	11198	26020	0.64%	0.181%
65	11.089	3023	3032	3043	rVB	7320	11225	0.28%	0.078%
66	11.166	3050	3056	3058	rBV2	293	302	0.01%	0.002%
67	11.237	3070	3078	3084	rVB6	1638	2375	0.06%	0.017%
68	11.292	3087	3095	3104	rBV	7768	11686	0.29%	0.081%
69	11.394	3123	3127	3130	rBV2	437	404	0.01%	0.003%
70	11.468	3139	3150	3166	rVB	42249	67278	1.66%	0.468%
71	11.607	3189	3193	3197	rVV5	362	398	0.01%	0.003%
72	11.700	3218	3222	3227	rBV4	347	351	0.01%	0.002%
73	11.742	3229	3235	3244	rBV6	2472	3353	0.08%	0.023%
74	11.812	3244	3257	3274	rBV	567805	895516	22.08%	6.234%
75	11.896	3274	3283	3292	rVB	16816	25577	0.63%	0.178%
76	11.970	3302	3306	3313	rVB4	1368	1442	0.04%	0.010%

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 Title : VOC Analysis

77	12.095	3336	3345	3352	rBV3	9804	15749	0.39%	0.110%
78	12.192	3364	3375	3393	rVB	324022	529594	13.06%	3.687%
79	12.378	3427	3433	3443	rVB	2502	3480	0.09%	0.024%
80	12.484	3455	3466	3486	rVV2	53222	101225	2.50%	0.705%
81	12.571	3486	3493	3502	rVV3	5355	7609	0.19%	0.053%
82	12.616	3505	3507	3516	rVB4	896	889	0.02%	0.006%
83	12.681	3522	3527	3529	rBV3	1018	952	0.02%	0.007%
84	12.774	3548	3556	3559	rBV3	1706	2046	0.05%	0.014%
85	12.880	3581	3589	3596	rVB4	1682	2363	0.06%	0.016%
86	12.951	3606	3611	3612	rBV4	1416	1168	0.03%	0.008%
87	13.025	3626	3634	3647	rVB3	3955	5595	0.14%	0.039%
88	13.111	3656	3661	3665	rBV4	436	509	0.01%	0.004%
89	13.166	3674	3678	3683	rBV2	354	368	0.01%	0.003%
90	13.221	3689	3695	3702	rVB6	2291	3046	0.08%	0.021%
91	13.298	3714	3719	3725	rVB5	935	1098	0.03%	0.008%
92	13.446	3759	3765	3781	rVB4	4686	7554	0.19%	0.053%
93	13.562	3797	3801	3802	rBV3	485	366	0.01%	0.003%
94	13.623	3817	3820	3826	rBV2	827	822	0.02%	0.006%
95	13.735	3852	3855	3863	rBV5	671	806	0.02%	0.006%
96	13.845	3881	3889	3902	rVB6	3672	5934	0.15%	0.041%
97	14.089	3954	3965	3980	rBV	34042	54839	1.35%	0.382%
98	14.330	4033	4040	4048	rBV5	3764	4897	0.12%	0.034%
99	15.227	4313	4319	4333	rVB3	4607	7125	0.18%	0.050%
100	15.603	4434	4436	4439	rBV4	766	396	0.01%	0.003%

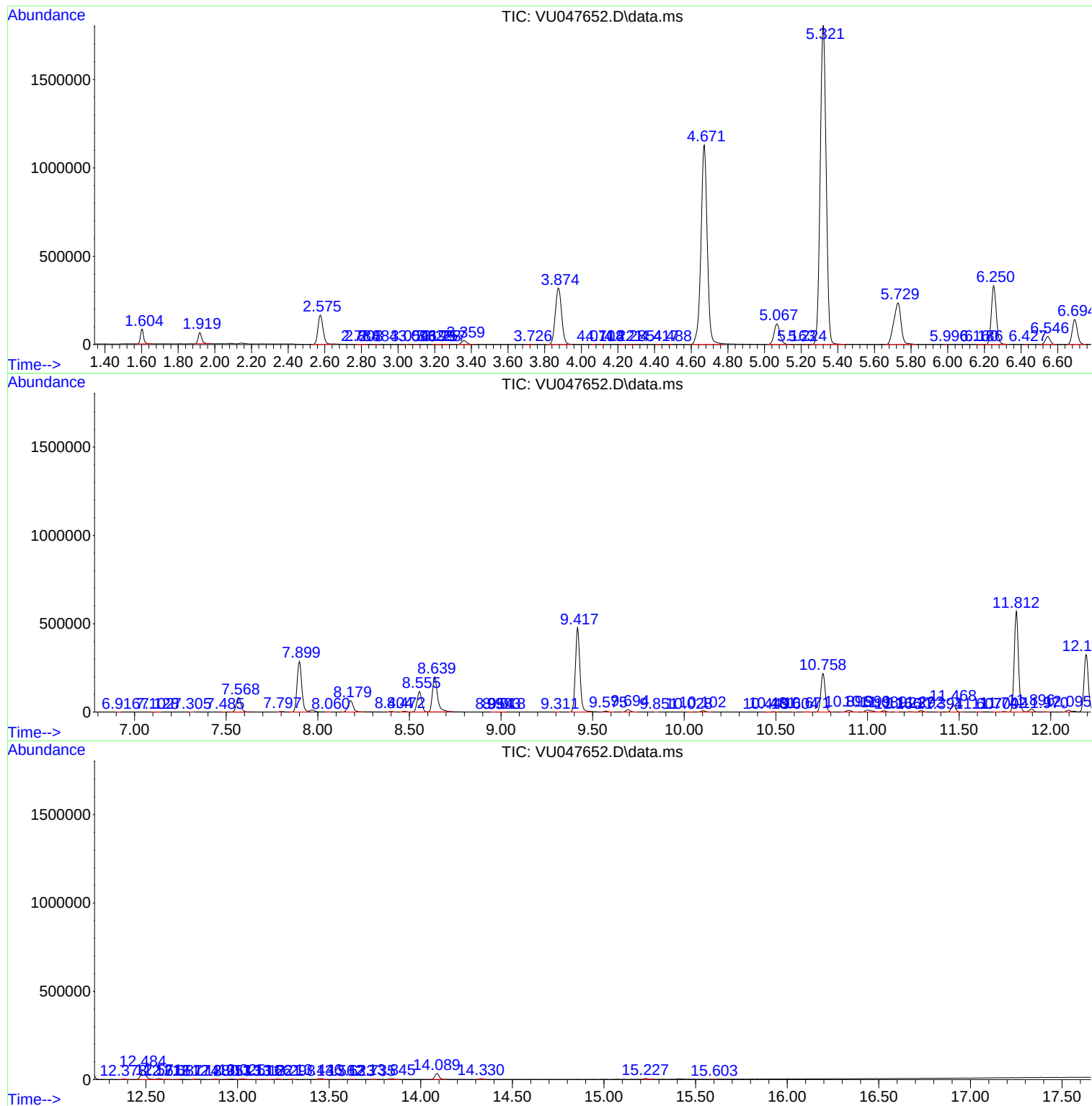
Sum of corrected areas: 14364579

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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



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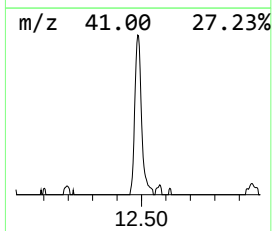
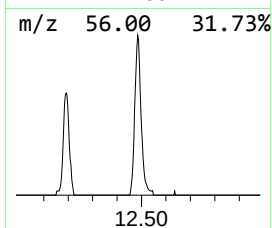
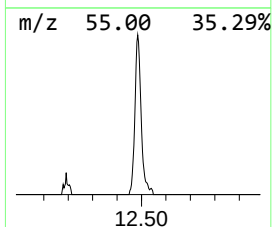
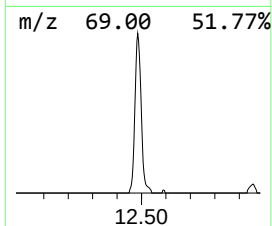
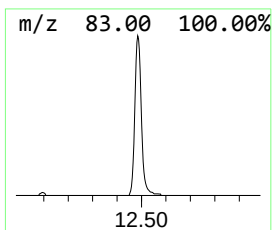
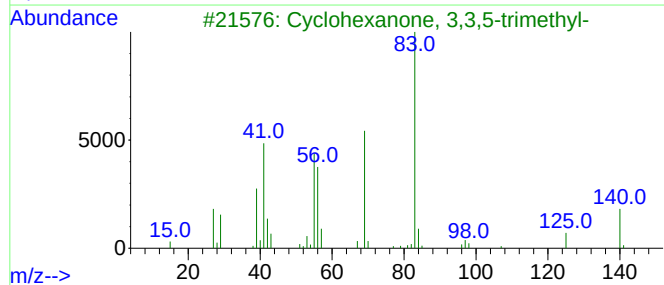
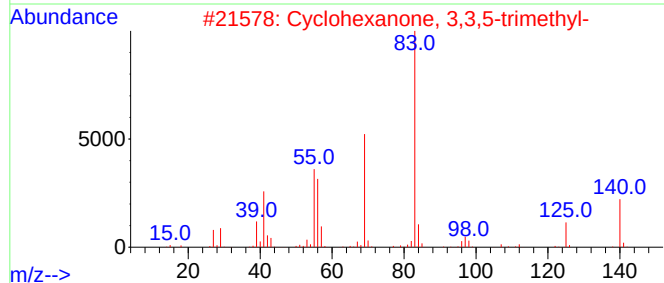
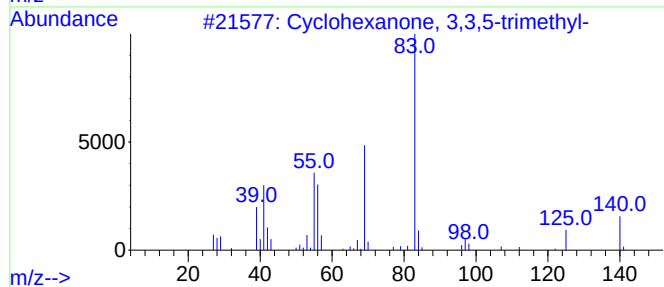
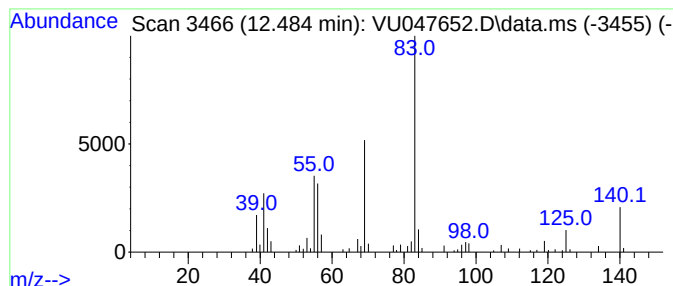
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Cyclohexanone, 3,3,5-trimet... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.485	5.65 ug/L	101225	1,4-Dichlorobenzene-d4	11.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	97
2			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	95
3			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	91
4			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	91
5			1,4-Pentadien-3-ol	84	C5H8O	000922-65-6	53



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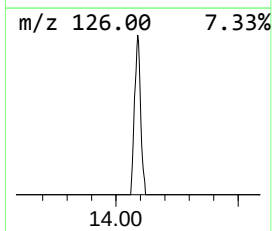
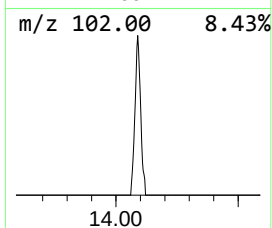
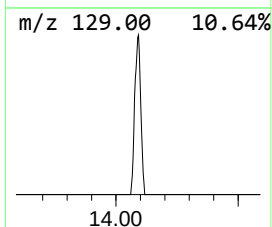
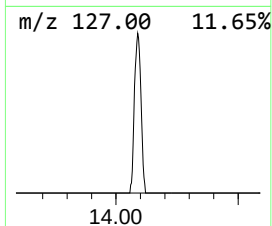
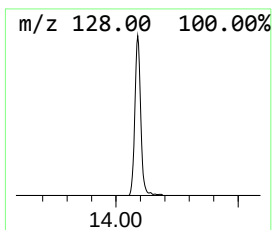
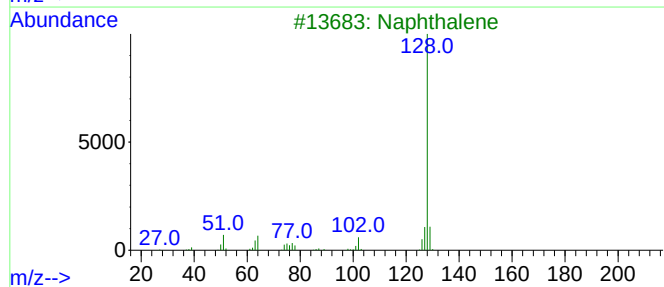
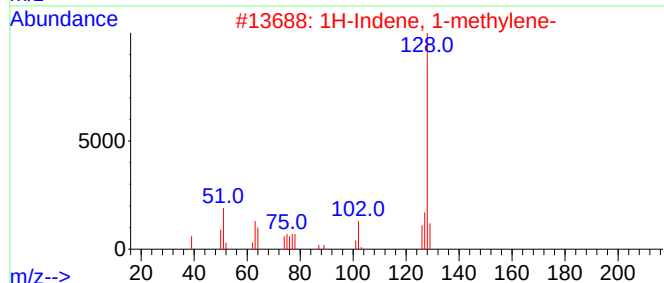
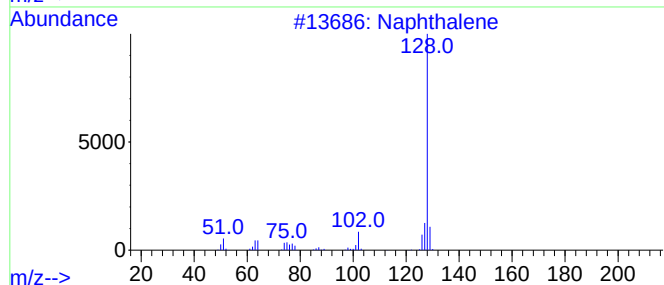
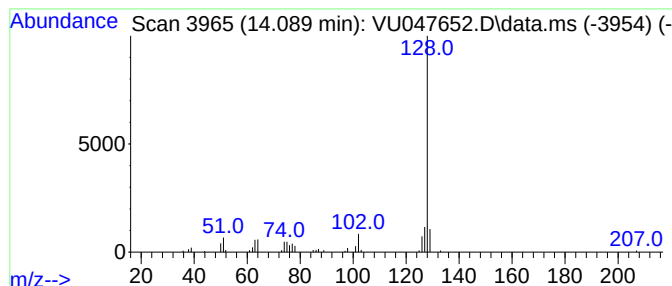
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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.
14.089	3.06 ug/L	54839	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 Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclohexanone, ...	12.485	5.7	ug/L	101225	3	11.813	895516	50.0
Azulene	14.089	3.1	ug/L	54839	3	11.813	895516	50.0