

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
 Data File : VU059325.D
 Acq On : 18 Jun 2024 20:42
 Operator : MD/SY
 Sample : P2873-12
 Misc : 5.41g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0SK0

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\SFAMULM052924WMA.M

Title : VOC Analysis

Signal : TIC: VU059325.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.480	55	59	65	rVB4	2402	2602	0.53%	0.059%
2	1.592	86	94	119	rVB	29810	57369	11.69%	1.303%
3	1.817	135	164	165	rBV4	41665	133234	27.16%	3.025%
4	2.489	371	373	376	rBV	396	289	0.06%	0.007%
5	2.534	376	387	404	rVB	86237	139159	28.37%	3.160%
6	2.682	431	433	438	rVB2	580	400	0.08%	0.009%
7	2.766	453	459	462	rVV2	507	638	0.13%	0.014%
8	2.817	472	475	478	rBV3	304	269	0.05%	0.006%
9	2.888	495	497	500	rBV2	502	332	0.07%	0.008%
10	3.026	527	540	552	rBV4	6421	13460	2.74%	0.306%
11	3.370	644	647	651	rVB2	386	275	0.06%	0.006%
12	3.396	651	655	660	rBV2	275	265	0.05%	0.006%
13	3.428	663	665	672	rVB2	223	214	0.04%	0.005%
14	3.544	695	701	703	rBV2	307	328	0.07%	0.007%
15	3.650	730	734	737	rBV2	262	248	0.05%	0.006%
16	3.676	737	742	745	rVV2	401	357	0.07%	0.008%
17	3.804	778	782	788	rBV2	338	364	0.07%	0.008%
18	4.039	850	855	857	rBV	268	319	0.07%	0.007%
19	4.177	893	898	901	rBV	271	270	0.06%	0.006%
20	4.213	906	909	912	rBV	338	274	0.06%	0.006%
21	4.258	918	923	926	rBV2	228	218	0.04%	0.005%
22	4.322	936	943	947	rBV	305	422	0.09%	0.010%
23	4.628	1028	1038	1068	rBV	41540	124418	25.36%	2.825%
24	4.862	1106	1111	1116	rBV3	351	462	0.09%	0.010%
25	5.052	1156	1170	1189	rVV2	84768	189402	38.61%	4.301%
26	5.171	1204	1207	1211	rVB3	306	237	0.05%	0.005%
27	5.444	1288	1292	1297	rBV	288	353	0.07%	0.008%
28	5.711	1357	1375	1402	rBV3	180397	472657	96.35%	10.733%
29	5.975	1449	1457	1469	rBV7	1567	3653	0.74%	0.083%
30	6.123	1500	1503	1508	rBV2	180	223	0.05%	0.005%
31	6.238	1527	1539	1566	rBV	195336	385058	78.49%	8.744%
32	6.389	1581	1586	1588	rBV2	293	271	0.06%	0.006%
33	6.528	1619	1629	1641	rVB9	4490	8763	1.79%	0.199%
34	6.598	1641	1651	1664	rBV3	2452	4983	1.02%	0.113%
35	6.682	1664	1677	1697	rBV2	108437	213377	43.50%	4.845%
36	6.898	1740	1744	1749	rBV	265	273	0.06%	0.006%

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Integrator: RTE

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
 Title : VOC Analysis

37	7.058	1790	1794	1799	rBV	361	458	0.09%	0.010%
38	7.200	1824	1838	1850	rBV6	1657	4092	0.83%	0.093%
39	7.242	1850	1851	1855	rVB2	357	223	0.05%	0.005%
40	7.364	1880	1889	1893	rBV2	274	520	0.11%	0.012%
41	7.560	1939	1950	1969	rBV2	50042	93588	19.08%	2.125%
42	7.698	1990	1993	1995	rBV2	538	358	0.07%	0.008%
43	7.711	1995	1997	2000	rVV4	393	230	0.05%	0.005%
44	7.756	2009	2011	2016	rBV2	347	222	0.05%	0.005%
45	7.891	2042	2053	2072	rBV	190649	342582	69.84%	7.779%
46	8.142	2125	2131	2132	rBV	247	206	0.04%	0.005%
47	8.177	2132	2142	2161	rVB2	33075	61854	12.61%	1.405%
48	8.457	2226	2229	2231	rVV2	367	256	0.05%	0.006%
49	8.473	2231	2234	2238	rVB2	272	263	0.05%	0.006%
50	8.547	2247	2257	2274	rBV2	47271	81398	16.59%	1.848%
51	8.640	2274	2286	2319	rBV	113219	265664	54.16%	6.033%
52	8.820	2339	2342	2347	rVB3	469	442	0.09%	0.010%
53	8.907	2364	2369	2373	rBV2	351	387	0.08%	0.009%
54	9.074	2415	2421	2424	rBV2	287	307	0.06%	0.007%
55	9.312	2493	2495	2499	rVB	307	215	0.04%	0.005%
56	9.351	2499	2507	2514	rBV2	244	556	0.11%	0.013%
57	9.415	2514	2527	2550	rBV	282461	490556	100.00%	11.139%
58	9.573	2569	2576	2584	rVB4	928	1306	0.27%	0.030%
59	9.676	2602	2608	2609	rBV2	394	371	0.08%	0.008%
60	9.701	2609	2616	2629	rVB4	2579	4263	0.87%	0.097%
61	10.106	2740	2742	2747	rVB3	583	432	0.09%	0.010%
62	10.341	2809	2815	2818	rBV	255	307	0.06%	0.007%
63	10.486	2856	2860	2863	rBV2	386	379	0.08%	0.009%
64	10.650	2906	2911	2914	rBV2	251	266	0.05%	0.006%
65	10.756	2932	2944	2969	rBV	179846	294032	59.94%	6.677%
66	10.884	2979	2984	2995	rBV2	880	1651	0.34%	0.037%
67	11.081	3041	3045	3046	rBV	486	301	0.06%	0.007%
68	11.274	3102	3105	3111	rBV2	216	246	0.05%	0.006%
69	11.306	3111	3115	3121	rVV2	281	336	0.07%	0.008%
70	11.409	3144	3147	3151	rVB	344	280	0.06%	0.006%
71	11.476	3162	3168	3173	rBV3	377	479	0.10%	0.011%
72	11.711	3238	3241	3248	rVB2	277	265	0.05%	0.006%
73	11.749	3248	3253	3259	rBV3	509	551	0.11%	0.013%
74	11.811	3260	3272	3297	rBV	295743	480844	98.02%	10.919%
75	11.968	3318	3321	3327	rVB2	358	342	0.07%	0.008%
76	12.190	3378	3390	3414	rBV	197227	332378	67.76%	7.547%

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 Title : VOC Analysis

77	12.476	3476	3479	3485	rBV2	290	316	0.06%	0.007%
78	12.505	3485	3488	3493	rBV2	183	208	0.04%	0.005%
79	12.769	3564	3570	3577	rVB2	831	1073	0.22%	0.024%
80	12.817	3582	3585	3588	rBV	284	231	0.05%	0.005%
81	12.904	3609	3612	3617	rBV2	245	278	0.06%	0.006%
82	13.257	3719	3722	3725	rBV	295	217	0.04%	0.005%
83	13.338	3744	3747	3749	rBV	287	205	0.04%	0.005%
84	13.402	3764	3767	3772	rVB	311	299	0.06%	0.007%
85	13.981	3944	3947	3949	rBV	334	217	0.04%	0.005%
86	14.087	3969	3980	4001	rBV	67790	121768	24.82%	2.765%
87	14.167	4001	4005	4009	rVB3	454	434	0.09%	0.010%
88	14.203	4014	4016	4018	rBV2	474	266	0.05%	0.006%
89	14.335	4053	4057	4060	rVB3	552	473	0.10%	0.011%
90	14.363	4063	4066	4069	rBV	317	211	0.04%	0.005%
91	14.550	4119	4124	4125	rBV2	455	373	0.08%	0.008%
92	14.637	4148	4151	4154	rBV2	286	226	0.05%	0.005%
93	15.225	4324	4334	4349	rBV2	16839	29021	5.92%	0.659%
94	15.412	4384	4392	4407	rVB2	7756	13209	2.69%	0.300%
95	15.945	4555	4558	4559	rBV2	741	443	0.09%	0.010%
96	16.154	4616	4623	4629	rBV5	1467	2521	0.51%	0.057%
97	16.251	4651	4653	4654	rBV3	727	357	0.07%	0.008%
98	16.273	4655	4660	4663	rVV3	2232	2151	0.44%	0.049%
99	16.412	4698	4703	4711	rVB5	2759	3335	0.68%	0.076%
100	17.100	4909	4917	4924	rBV4	4521	7203	1.47%	0.164%

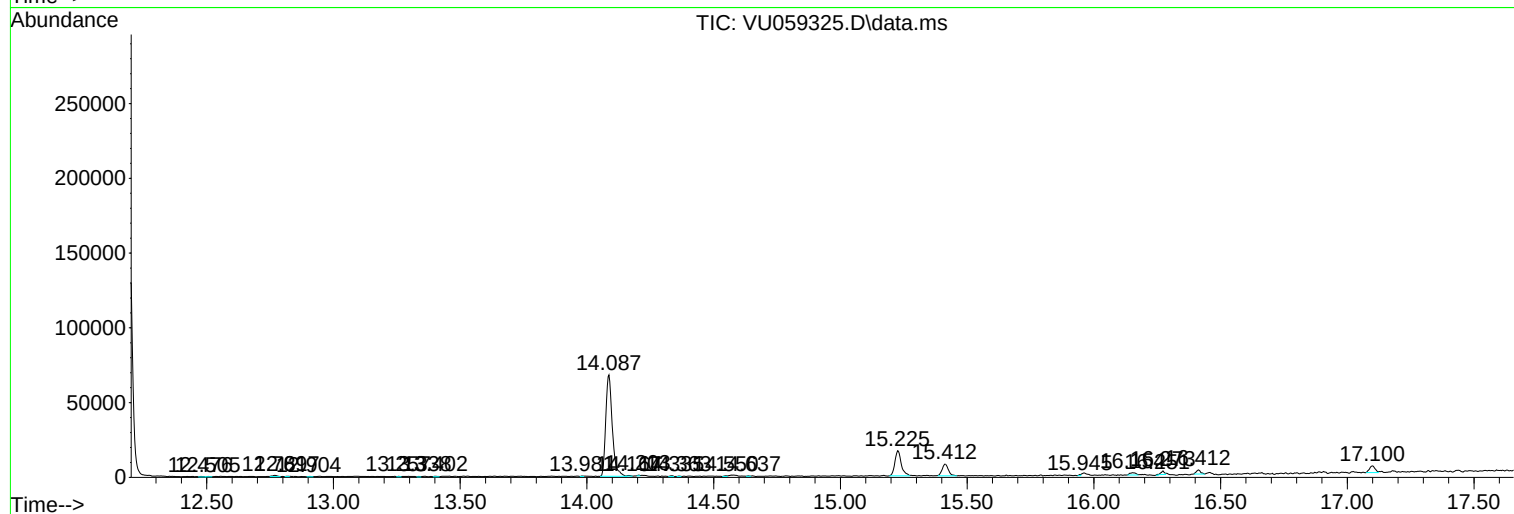
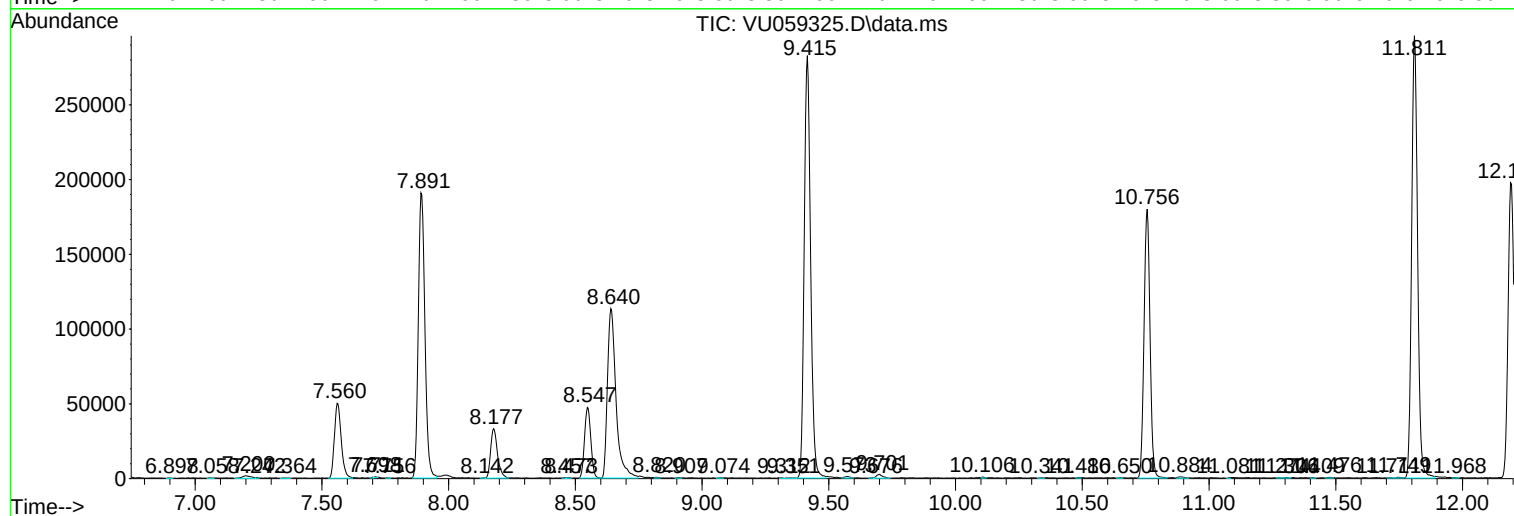
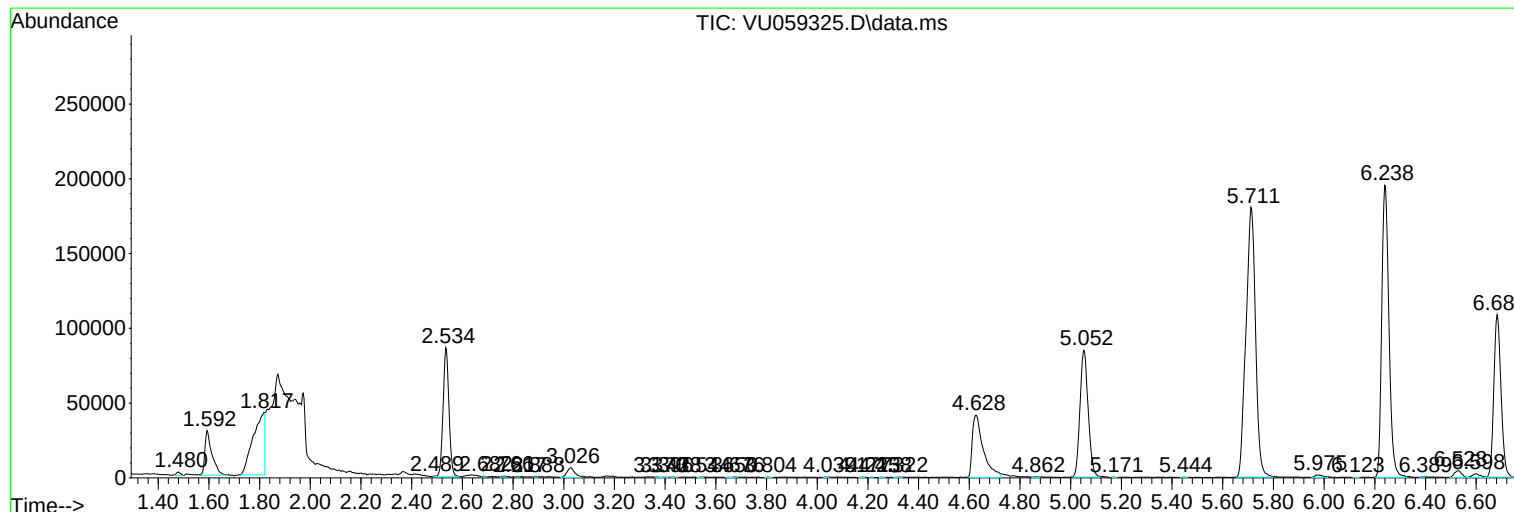
Sum of corrected areas: 4403877

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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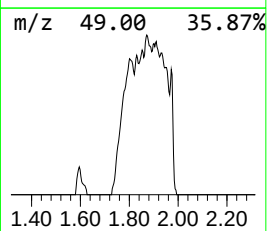
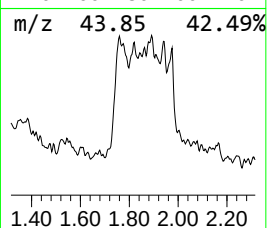
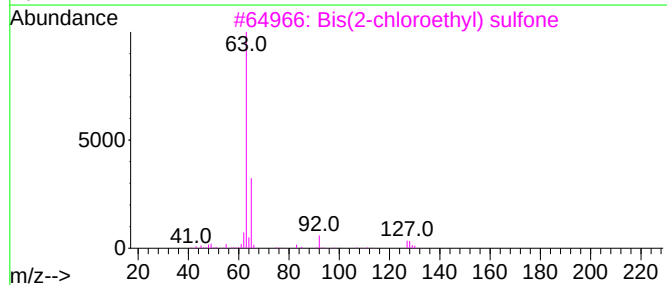
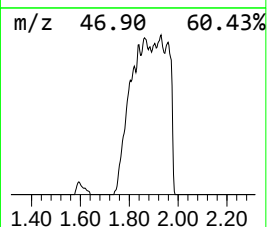
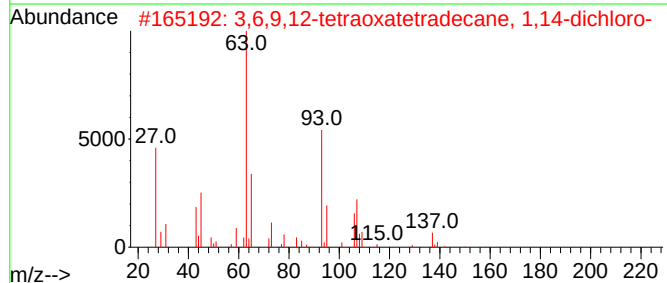
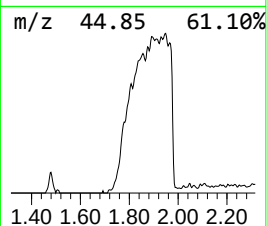
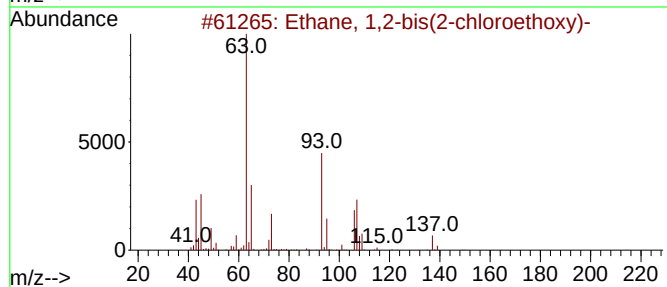
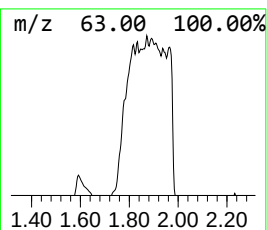
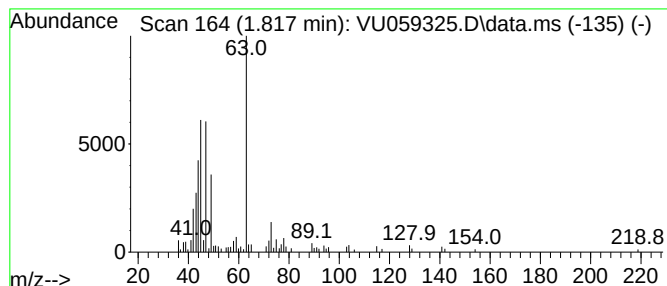
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.817	17.30 ug/L	133234	1,4-Difluorobenzene	6.238

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1,2-bis(2-chloroethoxy)-	186	C6H12Cl2O2	000112-26-5	33
2			3,6,9,12-tetraoxatetradecane, 1,...	274	C10H20Cl2O4	1000401-80-9	28
3			Bis(2-chloroethyl) sulfone	190	C4H8Cl2O2S	000471-03-4	28
4			Bis(2-chloroethyl) sulfone	190	C4H8Cl2O2S	000471-03-4	25
5			2-Chloropropionyl chloride	126	C3H4Cl2O	007623-09-8	25



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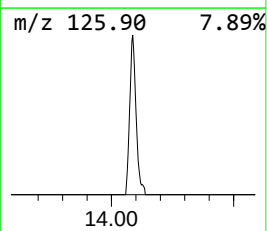
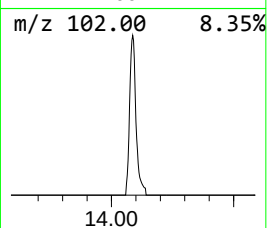
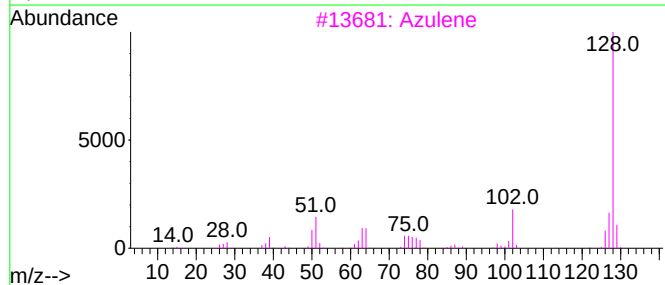
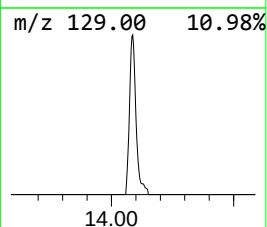
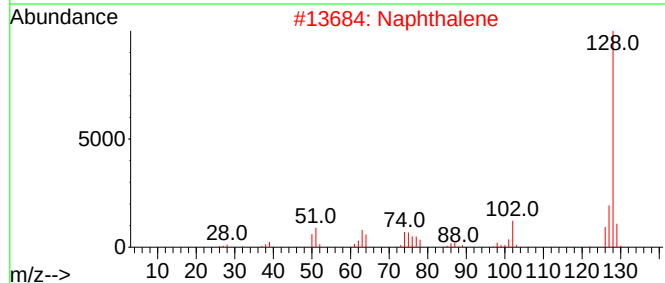
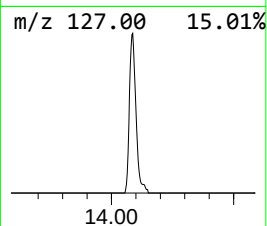
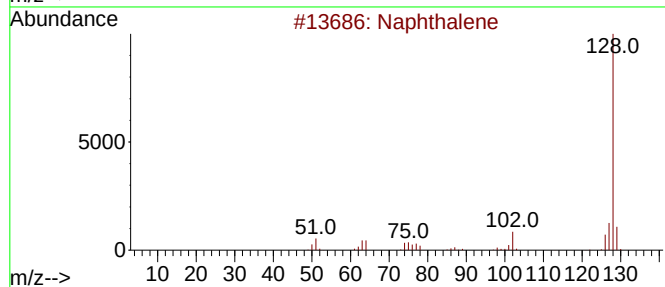
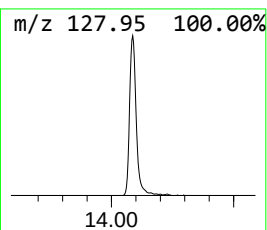
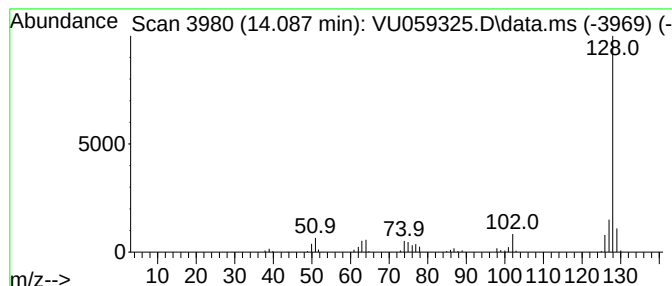
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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.
14.087	12.66 ug/L	121768	1,4-Dichlorobenzene-d4	11.810

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			Azulene	128	C10H8	000275-51-4	91
4			Azulene	128	C10H8	000275-51-4	91
5			Azulene	128	C10H8	000275-51-4	90



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Quant Title : VOC Analysis

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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.817	17.3	ug/L	133234	1	6.238	385058	50.0
Azulene	14.087	12.7	ug/L	121768	3	11.810	480844	50.0