

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062124\
 Data File : VU059410.D
 Acq On : 21 Jun 2024 13:56
 Operator : MD/SY
 Sample : P2962-15 100X
 Misc : 4.83g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 COT89

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: VU059410.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.595	87	95	111	rVB	58250	68383	9.84%	1.185%
2	1.763	139	147	162	rBV3	7784	12933	1.86%	0.224%
3	1.907	184	192	209	rVB	54682	75824	10.91%	1.314%
4	2.560	381	395	413	rBV	99697	162037	23.31%	2.808%
5	2.753	450	455	458	rBV2	467	480	0.07%	0.008%
6	3.039	534	544	555	rVB2	4681	9057	1.30%	0.157%
7	3.097	560	562	568	rVB2	344	245	0.04%	0.004%
8	3.300	619	625	629	rBV2	233	239	0.03%	0.004%
9	4.303	931	937	943	rBV2	242	333	0.05%	0.006%
10	4.402	965	968	970	rBV	289	231	0.03%	0.004%
11	4.534	1006	1009	1017	rVB	330	334	0.05%	0.006%
12	4.579	1017	1023	1024	rBV	310	267	0.04%	0.005%
13	4.615	1024	1034	1062	rBV	70432	177409	25.52%	3.074%
14	4.898	1119	1122	1125	rBV2	326	253	0.04%	0.004%
15	5.055	1154	1171	1197	rBV	111504	245269	35.29%	4.250%
16	5.148	1198	1200	1204	rVB3	409	257	0.04%	0.004%
17	5.316	1248	1252	1255	rBV2	322	231	0.03%	0.004%
18	5.505	1306	1311	1317	rBV2	404	633	0.09%	0.011%
19	5.718	1357	1377	1406	rBV2	214065	594693	85.56%	10.305%
20	5.898	1431	1433	1439	rVB3	499	347	0.05%	0.006%
21	5.936	1439	1445	1453	rBV3	458	623	0.09%	0.011%
22	6.000	1458	1465	1468	rBV	351	318	0.05%	0.006%
23	6.123	1500	1503	1510	rVB2	427	412	0.06%	0.007%
24	6.242	1528	1540	1566	rBV	285909	552275	79.45%	9.570%
25	6.531	1619	1630	1640	rVB3	4102	7363	1.06%	0.128%
26	6.685	1664	1678	1705	rBV	137677	275493	39.63%	4.774%
27	7.010	1776	1779	1783	rBV2	288	250	0.04%	0.004%
28	7.193	1829	1836	1837	rBV3	1577	1493	0.21%	0.026%
29	7.563	1940	1951	1973	rBV	67876	124265	17.88%	2.153%
30	7.701	1989	1994	1996	rBV	1000	872	0.13%	0.015%
31	7.894	2041	2054	2074	rBV	246197	425400	61.20%	7.372%
32	8.094	2113	2116	2122	rVB3	618	563	0.08%	0.010%
33	8.126	2122	2126	2128	rBV	360	251	0.04%	0.004%
34	8.177	2131	2142	2162	rBV	47067	82247	11.83%	1.425%
35	8.296	2175	2179	2181	rBV	338	271	0.04%	0.005%
36	8.547	2251	2257	2266	rVV6	2022	2888	0.42%	0.050%

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 Title : VOC Analysis

37	8.627	2271	2282	2312	rBV	189043	365887	52.64%	6.340%
38	8.846	2348	2350	2355	rVB3	316	248	0.04%	0.004%
39	9.168	2442	2450	2455	rBV2	351	427	0.06%	0.007%
40	9.328	2497	2500	2505	rBV2	303	271	0.04%	0.005%
41	9.412	2513	2526	2553	rBV	413914	695097	100.00%	12.045%
42	9.608	2584	2587	2592	rVB	327	260	0.04%	0.005%
43	9.701	2606	2616	2619	rBV3	761	1144	0.16%	0.020%
44	9.762	2632	2635	2639	rVB	397	302	0.04%	0.005%
45	9.962	2694	2697	2703	rBV2	284	250	0.04%	0.004%
46	10.106	2736	2742	2749	rBV3	322	458	0.07%	0.008%
47	10.203	2769	2772	2777	rBV2	207	268	0.04%	0.005%
48	10.251	2782	2787	2792	rVV3	697	848	0.12%	0.015%
49	10.386	2826	2829	2840	rBV3	516	732	0.11%	0.013%
50	10.553	2878	2881	2884	rBV2	410	334	0.05%	0.006%
51	10.621	2897	2902	2907	rVB4	882	952	0.14%	0.016%
52	10.749	2930	2942	2967	rVV	229946	376818	54.21%	6.530%
53	10.849	2970	2973	2977	rVB2	336	262	0.04%	0.005%
54	10.997	3015	3019	3020	rBV2	321	232	0.03%	0.004%
55	11.161	3065	3070	3076	rBV2	250	360	0.05%	0.006%
56	11.364	3130	3133	3135	rBV2	362	237	0.03%	0.004%
57	11.409	3142	3147	3155	rVB6	2199	3250	0.47%	0.056%
58	11.476	3163	3168	3169	rBV2	428	365	0.05%	0.006%
59	11.807	3259	3271	3296	rBV	399380	659988	94.95%	11.437%
60	11.997	3327	3330	3338	rBV5	913	1075	0.15%	0.019%
61	12.077	3352	3355	3357	rBV2	408	297	0.04%	0.005%
62	12.132	3364	3372	3376	rBV3	628	907	0.13%	0.016%
63	12.190	3377	3390	3420	rVV	262319	437760	62.98%	7.586%
64	12.412	3457	3459	3464	rVB	398	288	0.04%	0.005%
65	12.489	3480	3483	3488	rBV2	312	326	0.05%	0.006%
66	12.524	3491	3494	3497	rBV2	635	471	0.07%	0.008%
67	12.666	3532	3538	3541	rVB3	897	734	0.11%	0.013%
68	12.923	3614	3618	3620	rBV2	842	642	0.09%	0.011%
69	12.952	3625	3627	3633	rVB3	960	714	0.10%	0.012%
70	13.007	3639	3644	3647	rBV4	743	741	0.11%	0.013%
71	13.045	3654	3656	3660	rVB2	1008	663	0.10%	0.011%
72	13.135	3679	3684	3687	rBV3	721	672	0.10%	0.012%
73	13.425	3770	3774	3777	rBV3	422	361	0.05%	0.006%
74	13.454	3777	3783	3786	rBV4	734	888	0.13%	0.015%
75	13.531	3804	3807	3813	rVB3	836	634	0.09%	0.011%
76	13.582	3817	3823	3830	rVB5	3084	4189	0.60%	0.073%

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

77	13.978	3942	3946	3948	rBV3	656	523	0.08%	0.009%
78	14.000	3950	3953	3960	rVB5	819	783	0.11%	0.014%
79	14.039	3960	3965	3966	rBV3	1489	1092	0.16%	0.019%
80	14.087	3970	3980	3997	rVB	82026	141588	20.37%	2.454%
81	14.187	4006	4011	4018	rVB6	3276	4505	0.65%	0.078%
82	14.357	4060	4064	4065	rBV2	394	263	0.04%	0.005%
83	14.515	4110	4113	4114	rBV	643	314	0.05%	0.005%
84	14.560	4124	4127	4129	rBV2	703	572	0.08%	0.010%
85	14.630	4146	4149	4154	rBV4	1198	1368	0.20%	0.024%
86	14.875	4223	4225	4229	rVB2	627	393	0.06%	0.007%
87	14.965	4251	4253	4256	rBV2	457	242	0.03%	0.004%
88	15.064	4280	4284	4292	rVB6	1472	2038	0.29%	0.035%
89	15.138	4305	4307	4311	rBV3	370	292	0.04%	0.005%
90	15.222	4322	4333	4345	rBV	54280	94399	13.58%	1.636%
91	15.408	4381	4391	4404	rBV	27495	45399	6.53%	0.787%
92	15.958	4554	4562	4576	rVB4	8861	15037	2.16%	0.261%
93	16.039	4585	4587	4591	rVB4	1290	697	0.10%	0.012%
94	16.145	4613	4620	4628	rBV3	4963	7190	1.03%	0.125%
95	16.187	4628	4633	4642	rVB6	4338	5251	0.76%	0.091%
96	16.260	4649	4656	4669	rBV4	10466	19302	2.78%	0.334%
97	16.408	4693	4702	4709	rBV4	12469	20103	2.89%	0.348%
98	16.537	4739	4742	4743	rBV4	1971	1242	0.18%	0.022%
99	16.785	4814	4819	4826	rBV8	2654	3719	0.54%	0.064%
100	16.884	4843	4850	4864	rVB2	11814	19682	2.83%	0.341%

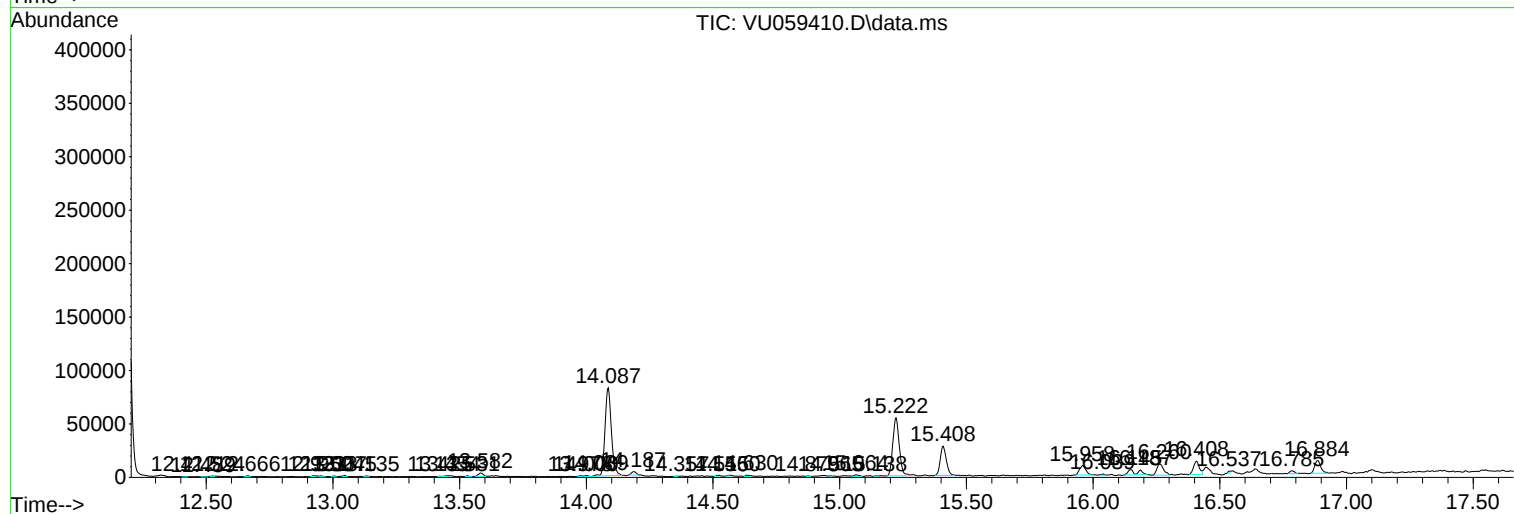
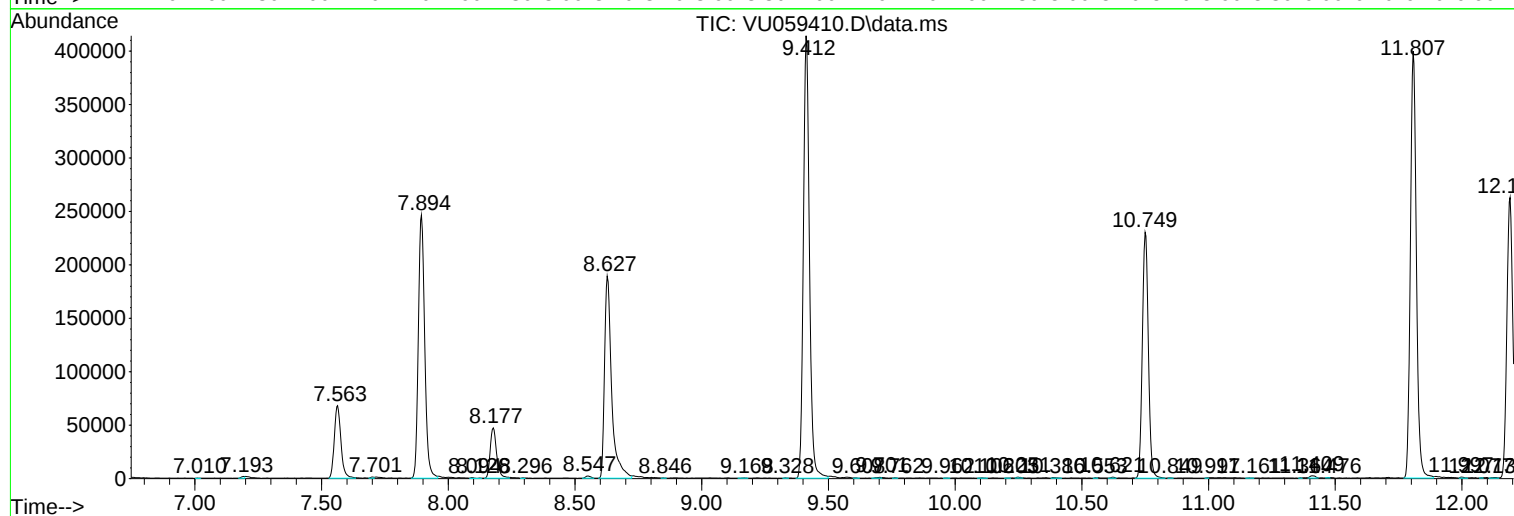
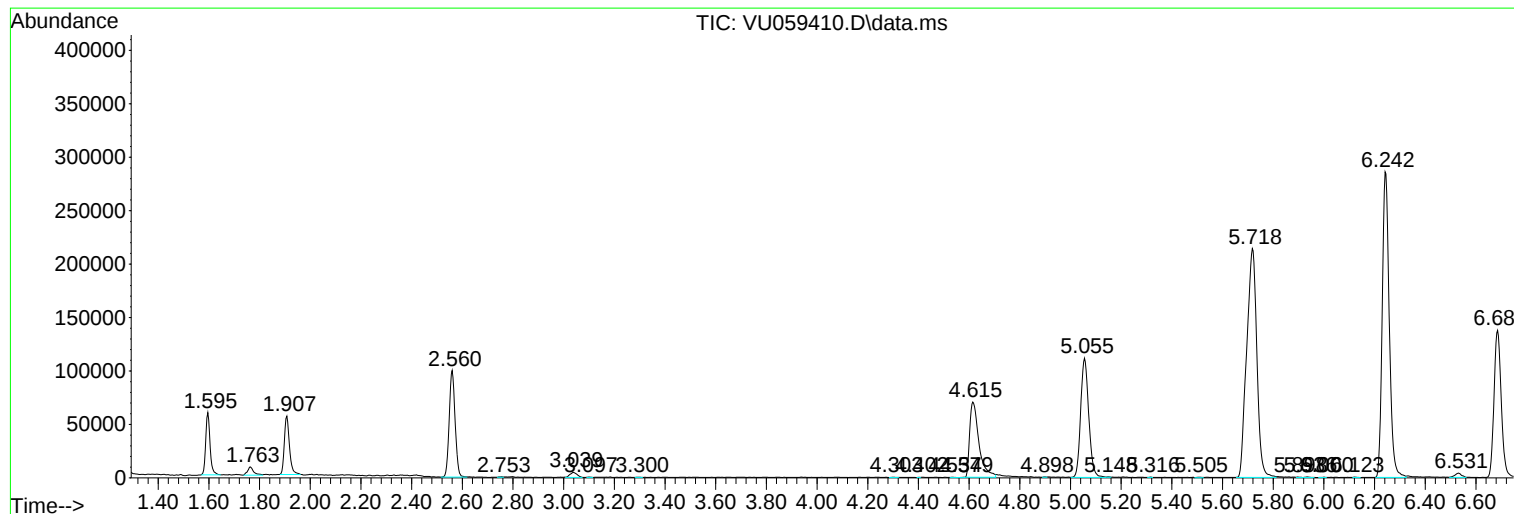
Sum of corrected areas: 5770785

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Instrument :
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ClientSampleId :
C0T89

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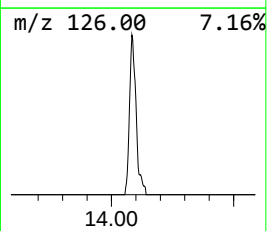
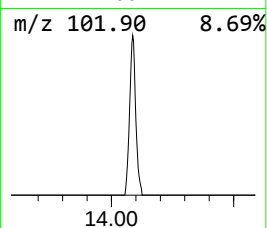
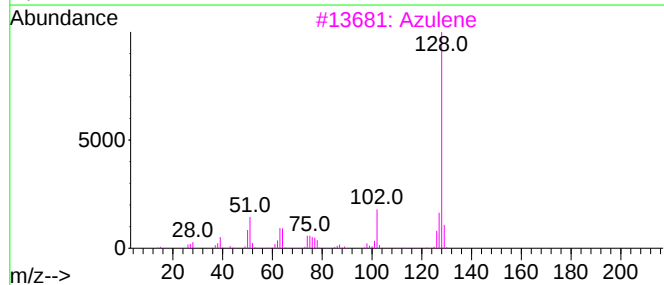
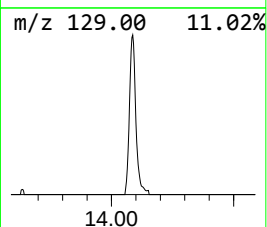
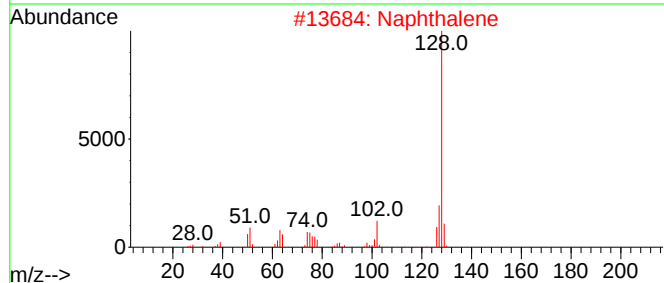
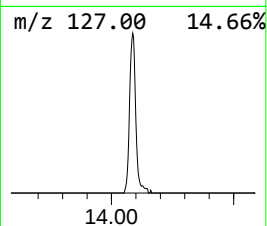
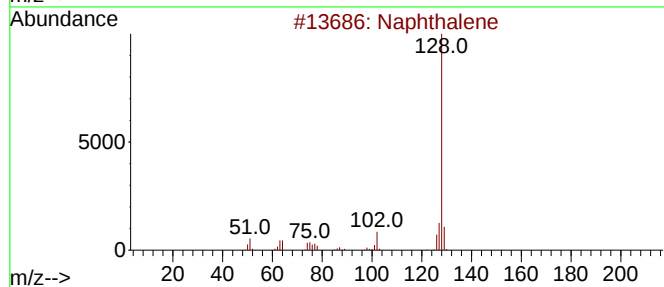
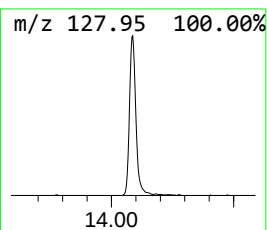
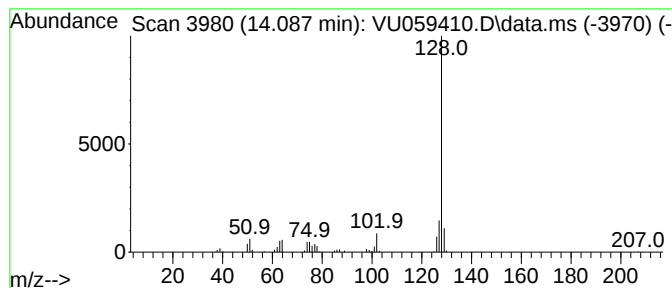
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Azulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.087	10.73 ug/L	141588	1,4-Dichlorobenzene-d4	11.807

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	90
5			Azulene	128	C10H8	000275-51-4	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Azulene	14.087	10.7	ug/L	141588	3	11.807	659988	50.0