

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061424\
 Data File : VU059262.D
 Acq On : 14 Jun 2024 20:49
 Operator : MD/SY
 Sample : P2798-05ME
 Misc : 5.27g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHB16ME

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: VU059262.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	56	59	64	rVB2	1700	1594	0.23%	0.023%
2	1.592	87	94	118	rVB	31380	52643	7.63%	0.767%
3	1.837	136	170	172	rBV4	54001	220881	32.01%	3.218%
4	2.493	370	374	377	rBV2	460	356	0.05%	0.005%
5	2.541	377	389	403	rBV	86407	137984	20.00%	2.010%
6	2.608	408	410	412	rBV2	413	240	0.03%	0.003%
7	2.685	432	434	437	rVB	453	258	0.04%	0.004%
8	2.772	457	461	466	rVV2	582	638	0.09%	0.009%
9	3.029	530	541	556	rBV3	5804	12188	1.77%	0.178%
10	3.174	573	586	604	rBV2	7076	18579	2.69%	0.271%
11	3.341	634	638	640	rBV2	292	237	0.03%	0.003%
12	3.480	678	681	687	rBV	260	332	0.05%	0.005%
13	3.673	735	741	746	rBV2	465	520	0.08%	0.008%
14	3.775	770	773	779	rVB	197	208	0.03%	0.003%
15	3.817	779	786	790	rBV	193	323	0.05%	0.005%
16	3.856	795	798	802	rVV	232	201	0.03%	0.003%
17	4.412	964	971	975	rBV2	384	504	0.07%	0.007%
18	4.496	995	997	1008	rVB2	188	317	0.05%	0.005%
19	4.650	1025	1045	1086	rBV3	204869	690037	100.00%	10.053%
20	4.972	1140	1145	1147	rBV3	297	307	0.04%	0.004%
21	5.052	1153	1170	1193	rBV	124773	282761	40.98%	4.119%
22	5.148	1197	1200	1205	rVB2	446	457	0.07%	0.007%
23	5.412	1274	1282	1288	rBV2	212	298	0.04%	0.004%
24	5.711	1353	1375	1408	rBV2	225171	615939	89.26%	8.973%
25	5.920	1434	1440	1444	rBV3	269	289	0.04%	0.004%
26	5.975	1452	1457	1462	rBV4	916	1201	0.17%	0.017%
27	6.116	1495	1501	1507	rBV3	391	536	0.08%	0.008%
28	6.238	1527	1539	1575	rBV	268719	525019	76.09%	7.649%
29	6.534	1618	1631	1644	rBV7	13105	27944	4.05%	0.407%
30	6.592	1644	1649	1651	rBV3	941	929	0.13%	0.014%
31	6.682	1664	1677	1705	rVB	162947	322360	46.72%	4.696%
32	6.814	1713	1718	1720	rBV2	436	319	0.05%	0.005%
33	6.975	1763	1768	1772	rBV2	196	223	0.03%	0.003%
34	7.193	1831	1836	1850	rBV7	967	2203	0.32%	0.032%
35	7.322	1872	1876	1879	rBV	416	335	0.05%	0.005%
36	7.502	1929	1932	1935	rBV2	312	201	0.03%	0.003%

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Integration Parameters: LSCINT.P

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	7.560	1938	1950	1968	rBV	73688	134806	19.54%	1.964%
38	7.666	1980	1983	1987	rBV2	351	306	0.04%	0.004%
39	7.705	1987	1995	2008	rVV4	1051	2073	0.30%	0.030%
40	7.891	2041	2053	2074	rBV	229219	404238	58.58%	5.889%
41	8.081	2107	2112	2115	rVB4	325	324	0.05%	0.005%
42	8.174	2131	2141	2165	rVV	49371	91513	13.26%	1.333%
43	8.364	2197	2200	2208	rBV2	263	354	0.05%	0.005%
44	8.473	2227	2234	2238	rBV3	522	553	0.08%	0.008%
45	8.547	2246	2257	2272	rVB2	66198	113922	16.51%	1.660%
46	8.637	2272	2285	2320	rBV	252727	607358	88.02%	8.848%
47	8.827	2341	2344	2346	rBV4	543	311	0.05%	0.005%
48	8.968	2384	2388	2389	rBV	252	202	0.03%	0.003%
49	9.148	2441	2444	2448	rVB	316	252	0.04%	0.004%
50	9.171	2448	2451	2454	rBV2	368	278	0.04%	0.004%
51	9.270	2476	2482	2484	rBV2	267	273	0.04%	0.004%
52	9.412	2514	2526	2551	rBV	389946	682953	98.97%	9.949%
53	9.695	2606	2614	2618	rBV3	1387	1853	0.27%	0.027%
54	9.785	2639	2642	2647	rVV	446	371	0.05%	0.005%
55	9.991	2702	2706	2709	rVV2	243	207	0.03%	0.003%
56	10.106	2733	2742	2745	rVV4	781	957	0.14%	0.014%
57	10.151	2754	2756	2760	rBV	352	312	0.05%	0.005%
58	10.196	2764	2770	2772	rBV2	225	238	0.03%	0.003%
59	10.248	2778	2786	2794	rVV4	1289	1933	0.28%	0.028%
60	10.389	2823	2830	2836	rBV3	899	940	0.14%	0.014%
61	10.486	2854	2860	2862	rBV3	329	337	0.05%	0.005%
62	10.553	2873	2881	2884	rBV3	783	852	0.12%	0.012%
63	10.592	2889	2893	2894	rBV	411	278	0.04%	0.004%
64	10.618	2896	2901	2907	rBV5	1418	1671	0.24%	0.024%
65	10.753	2930	2943	2969	rVV	359787	589979	85.50%	8.595%
66	10.888	2981	2985	2987	rBV3	405	315	0.05%	0.005%
67	10.994	3014	3018	3022	rVB	328	252	0.04%	0.004%
68	11.061	3035	3039	3040	rBV	363	258	0.04%	0.004%
69	11.119	3055	3057	3059	rVB	496	254	0.04%	0.004%
70	11.306	3108	3115	3116	rBV2	254	272	0.04%	0.004%
71	11.415	3141	3149	3154	rBV3	2713	3595	0.52%	0.052%
72	11.630	3212	3216	3219	rBV2	334	238	0.03%	0.003%
73	11.704	3233	3239	3246	rVB4	849	1099	0.16%	0.016%
74	11.749	3246	3253	3255	rBV2	839	674	0.10%	0.010%
75	11.807	3260	3271	3292	rBV	390189	646274	93.66%	9.415%
76	11.926	3306	3308	3314	rVB5	608	461	0.07%	0.007%

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Instrument :
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 ClientSampleId :
 BHB16ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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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

77	12.190	3377	3390	3417	rBV	327382	541489	78.47%	7.889%
78	12.331	3431	3434	3436	rBV2	439	218	0.03%	0.003%
79	12.367	3441	3445	3447	rBV3	334	219	0.03%	0.003%
80	12.399	3452	3455	3460	rVB2	459	295	0.04%	0.004%
81	12.569	3504	3508	3516	rBV2	290	353	0.05%	0.005%
82	12.730	3554	3558	3561	rBV2	463	293	0.04%	0.004%
83	12.769	3561	3570	3577	rVV4	1061	1629	0.24%	0.024%
84	13.264	3720	3724	3728	rBV2	533	620	0.09%	0.009%
85	13.843	3902	3904	3907	rVB	483	247	0.04%	0.004%
86	13.968	3940	3943	3948	rBV	346	254	0.04%	0.004%
87	14.013	3955	3957	3962	rVB2	401	272	0.04%	0.004%
88	14.087	3968	3980	4005	rBV	50952	100318	14.54%	1.461%
89	14.244	4027	4029	4032	rBV	415	217	0.03%	0.003%
90	14.566	4125	4129	4137	rVB3	987	1504	0.22%	0.022%
91	14.653	4152	4156	4158	rBV	357	294	0.04%	0.004%
92	14.746	4180	4185	4187	rBV2	362	340	0.05%	0.005%
93	14.859	4218	4220	4226	rVB2	362	327	0.05%	0.005%
94	14.987	4257	4260	4265	rBV	345	344	0.05%	0.005%
95	15.103	4292	4296	4299	rBV2	609	410	0.06%	0.006%
96	15.283	4349	4352	4355	rBV3	351	339	0.05%	0.005%
97	15.614	4452	4455	4457	rBV2	451	256	0.04%	0.004%
98	15.733	4490	4492	4498	rBV2	528	359	0.05%	0.005%
99	16.164	4623	4626	4630	rBV4	619	559	0.08%	0.008%
100	16.232	4644	4647	4648	rBV2	688	387	0.06%	0.006%

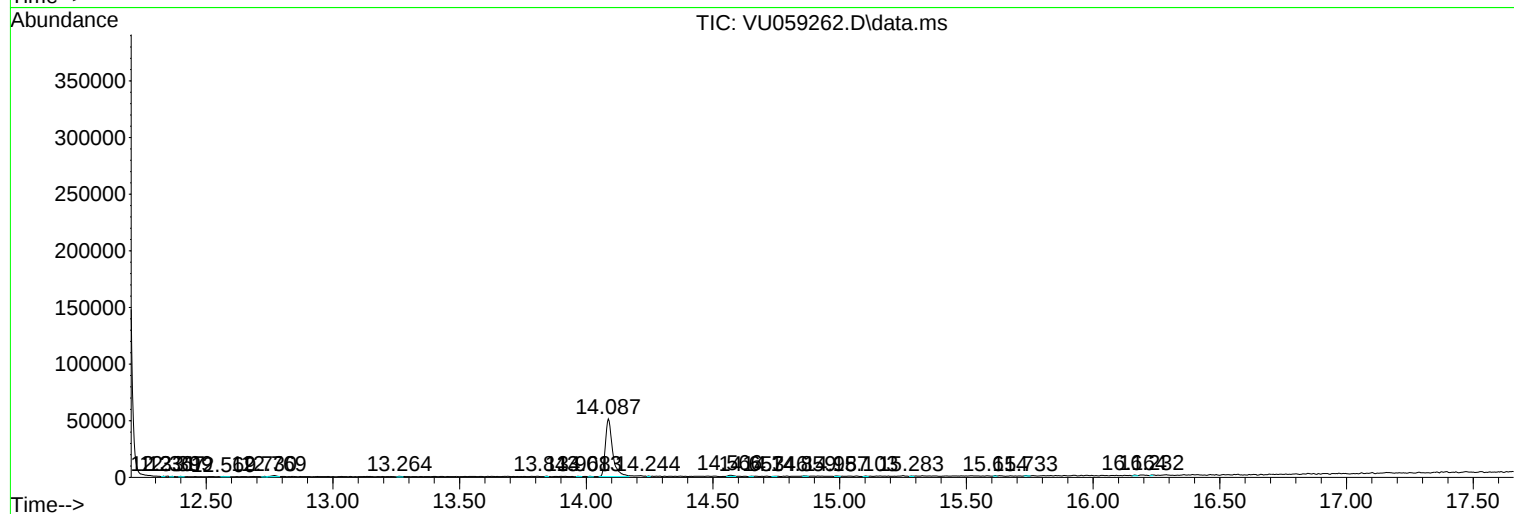
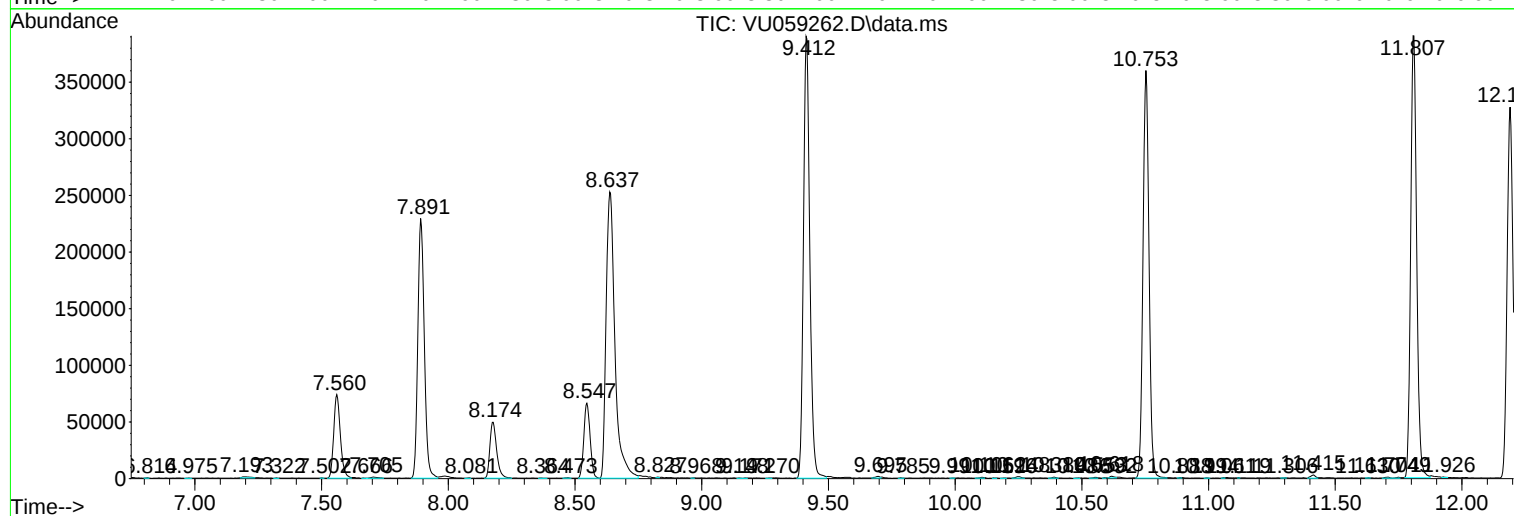
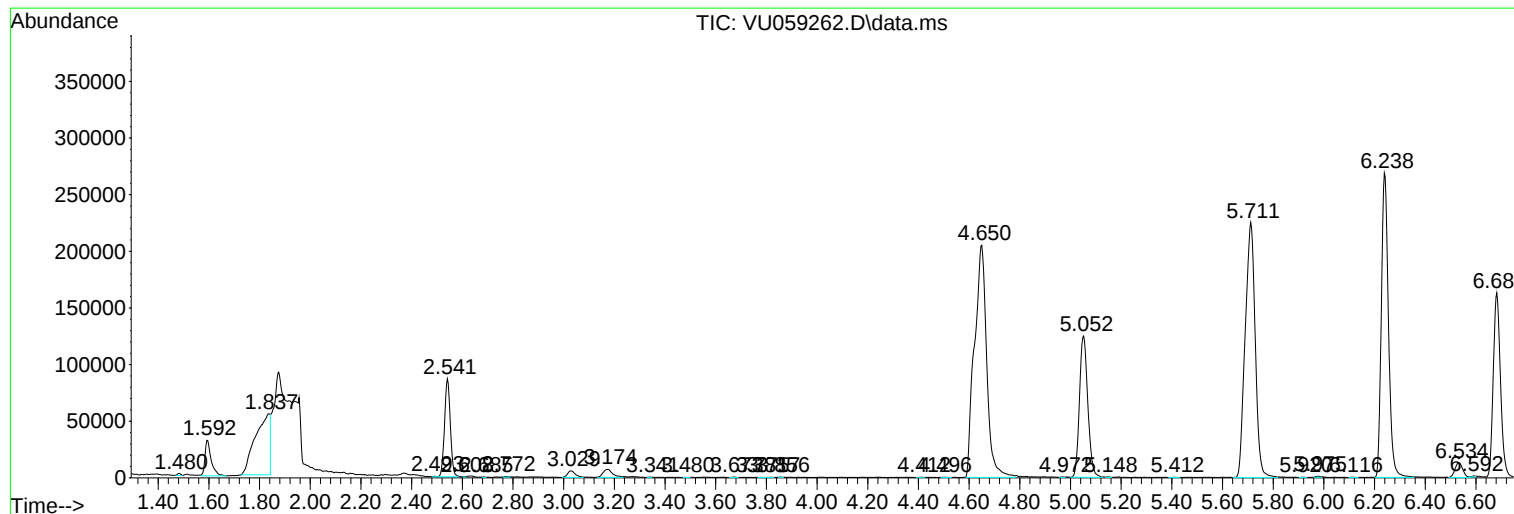
Sum of corrected areas: 6864240

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ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleId :
BHB16ME

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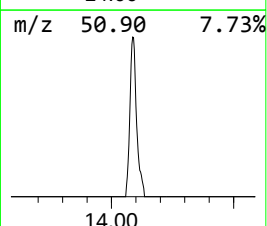
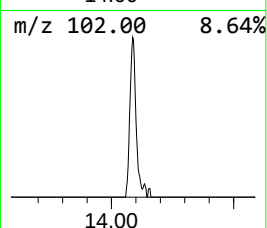
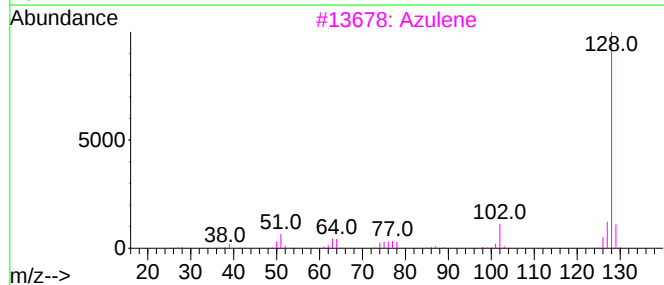
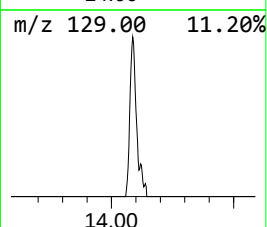
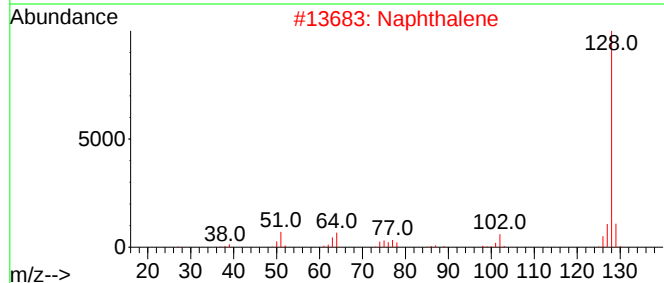
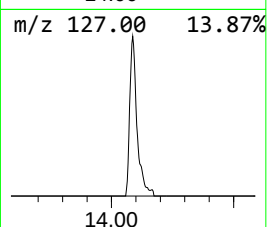
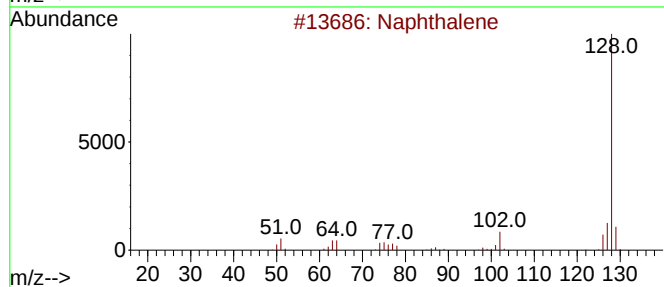
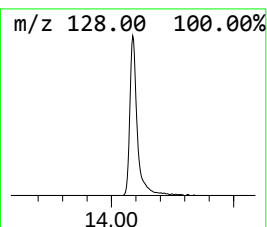
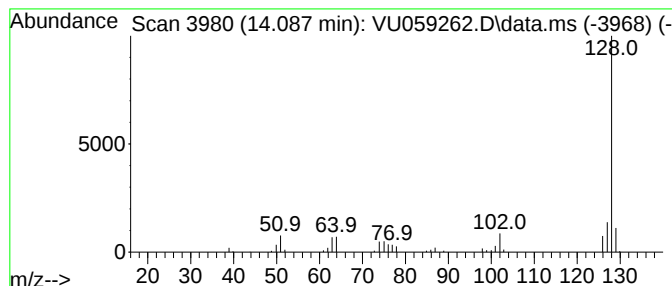
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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	7.76 ug/L	100318	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	95
3			Azulene	128	C10H8	000275-51-4	94
4			Naphthalene	128	C10H8	000091-20-3	94
5			Naphthalene	128	C10H8	000091-20-3	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Azulene	14.087	7.8	ug/L	100318	3	11.810	646274	50.0