

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
 Data File : VU059313.D
 Acq On : 18 Jun 2024 15:36
 Operator : MD/SY
 Sample : P2897-08 100X
 Misc : 4.18g/5.0mL/100uL/5.1mL/MSVOA_U/MEOH
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0SL3

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: VU059313.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.596	87	95	112	rVB	50478	59992	10.84%	1.074%
2	1.766	139	148	161	rBV	10057	14368	2.60%	0.257%
3	1.908	184	192	212	rVB	45705	63489	11.47%	1.137%
4	2.490	371	373	378	rBV2	380	255	0.05%	0.005%
5	2.560	382	395	411	rBV	81769	133647	24.15%	2.394%
6	2.753	447	455	459	rBV3	481	471	0.09%	0.008%
7	2.782	459	464	470	rBV3	337	511	0.09%	0.009%
8	2.856	484	487	492	rVB2	235	258	0.05%	0.005%
9	3.040	533	544	561	rBV3	15377	31012	5.60%	0.555%
10	3.178	581	587	592	rVB3	469	548	0.10%	0.010%
11	3.525	692	695	702	rVB2	404	462	0.08%	0.008%
12	3.564	702	707	712	rBV2	294	386	0.07%	0.007%
13	3.853	792	797	802	rBV	203	253	0.05%	0.005%
14	4.265	919	925	928	rBV	300	348	0.06%	0.006%
15	4.290	928	933	935	rBV	244	251	0.05%	0.004%
16	4.615	1022	1034	1061	rBV	46347	118053	21.33%	2.114%
17	4.805	1087	1093	1096	rBV3	315	297	0.05%	0.005%
18	5.056	1153	1171	1191	rBV	82449	182939	33.05%	3.276%
19	5.605	1339	1342	1347	rVB3	264	261	0.05%	0.005%
20	5.718	1354	1377	1403	rBV2	164988	453320	81.90%	8.119%
21	5.940	1442	1446	1452	rBV2	292	452	0.08%	0.008%
22	6.242	1528	1540	1567	rBV	200681	393615	71.11%	7.050%
23	6.525	1620	1628	1639	rVV5	3167	6021	1.09%	0.108%
24	6.686	1665	1678	1700	rBV	106602	208296	37.63%	3.731%
25	6.869	1731	1735	1740	rBV2	373	397	0.07%	0.007%
26	7.194	1831	1836	1840	rBV3	1172	1243	0.22%	0.022%
27	7.297	1863	1868	1870	rBV	274	260	0.05%	0.005%
28	7.564	1940	1951	1971	rBV2	47456	85500	15.45%	1.531%
29	7.705	1989	1995	2000	rBV4	911	934	0.17%	0.017%
30	7.895	2041	2054	2072	rBV	182316	318792	57.60%	5.709%
31	8.104	2115	2119	2121	rVB2	379	275	0.05%	0.005%
32	8.178	2131	2142	2158	rBV	33076	57112	10.32%	1.023%
33	8.300	2177	2180	2189	rBV2	213	328	0.06%	0.006%
34	8.547	2244	2257	2273	rBV2	304111	514598	92.97%	9.216%
35	8.628	2273	2282	2310	rVV	117413	224251	40.52%	4.016%
36	8.814	2336	2340	2342	rVB3	514	308	0.06%	0.006%

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

37	8.862	2352	2355	2360	rVB2	327	289	0.05%	0.005%
38	9.010	2394	2401	2409	rBV2	265	580	0.10%	0.010%
39	9.123	2434	2436	2443	rBV2	242	286	0.05%	0.005%
40	9.412	2513	2526	2549	rBV	296522	509227	92.00%	9.120%
41	9.570	2567	2575	2587	rVB	5000	7913	1.43%	0.142%
42	9.692	2602	2613	2624	rBV2	13884	23325	4.21%	0.418%
43	9.782	2638	2641	2647	rVB2	434	413	0.07%	0.007%
44	9.821	2647	2653	2655	rBV	306	301	0.05%	0.005%
45	10.100	2730	2740	2755	rBV4	5234	9932	1.79%	0.178%
46	10.489	2856	2861	2866	rVB	1148	1147	0.21%	0.021%
47	10.531	2866	2874	2876	rBV	334	450	0.08%	0.008%
48	10.750	2930	2942	2958	rBV	159003	257884	46.59%	4.619%
49	10.830	2964	2967	2971	rVB2	357	251	0.05%	0.004%
50	10.907	2989	2991	3003	rVB3	933	1180	0.21%	0.021%
51	11.001	3009	3020	3026	rBV3	5956	10459	1.89%	0.187%
52	11.087	3036	3047	3057	rBV2	7088	10892	1.97%	0.195%
53	11.290	3105	3110	3111	rBV3	993	769	0.14%	0.014%
54	11.325	3119	3121	3130	rVB3	1143	846	0.15%	0.015%
55	11.467	3155	3165	3178	rVB2	20105	31220	5.64%	0.559%
56	11.538	3178	3187	3196	rVV	15514	23591	4.26%	0.423%
57	11.589	3199	3203	3214	rVB5	4001	5566	1.01%	0.100%
58	11.653	3220	3223	3228	rBV3	296	309	0.06%	0.006%
59	11.734	3242	3248	3250	rBV2	353	359	0.06%	0.006%
60	11.808	3259	3271	3290	rBV	294565	483654	87.38%	8.662%
61	11.895	3290	3298	3310	rVV3	6556	11026	1.99%	0.197%
62	11.956	3310	3317	3330	rVB2	2526	4704	0.85%	0.084%
63	12.007	3330	3333	3337	rBV2	310	285	0.05%	0.005%
64	12.094	3351	3360	3366	rBV4	3013	4737	0.86%	0.085%
65	12.190	3378	3390	3408	rBV	192580	314554	56.83%	5.634%
66	12.313	3417	3428	3446	rVB3	15332	26554	4.80%	0.476%
67	12.380	3446	3449	3453	rBV	367	328	0.06%	0.006%
68	12.499	3483	3486	3491	rVB3	1085	803	0.15%	0.014%
69	12.570	3496	3508	3516	rBV6	1651	3425	0.62%	0.061%
70	12.747	3554	3563	3577	rVB5	4839	8132	1.47%	0.146%
71	12.817	3578	3585	3590	rVB4	991	1408	0.25%	0.025%
72	12.846	3590	3594	3597	rBV	297	299	0.05%	0.005%
73	12.978	3626	3635	3640	rBV3	1023	1152	0.21%	0.021%
74	13.026	3643	3650	3658	rBV5	2696	4113	0.74%	0.074%
75	13.152	3683	3689	3700	rBV6	2462	4158	0.75%	0.074%
76	13.293	3726	3733	3740	rBV3	785	1029	0.19%	0.018%

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77	13.444	3768	3780	3789	rVB9	2523	5029	0.91%	0.090%
78	13.518	3794	3803	3813	rVV3	8798	13202	2.39%	0.236%
79	13.628	3825	3837	3851	rVB2	9106	15758	2.85%	0.282%
80	13.730	3863	3869	3877	rVB4	1570	1869	0.34%	0.033%
81	13.866	3907	3911	3917	rVB2	260	262	0.05%	0.005%
82	14.081	3962	3978	4006	rBV	326254	553500	100.00%	9.913%
83	14.206	4013	4017	4029	rVB3	2654	4037	0.73%	0.072%
84	14.447	4087	4092	4097	rVV5	1110	1422	0.26%	0.025%
85	14.489	4101	4105	4109	rBV3	618	628	0.11%	0.011%
86	14.570	4123	4130	4131	rBV4	1097	980	0.18%	0.018%
87	14.679	4155	4164	4169	rBV5	1734	2528	0.46%	0.045%
88	14.721	4175	4177	4183	rVB2	496	411	0.07%	0.007%
89	14.804	4191	4203	4214	rVB6	1858	3896	0.70%	0.070%
90	15.004	4262	4265	4267	rBV2	472	362	0.07%	0.006%
91	15.071	4282	4286	4290	rBV3	886	882	0.16%	0.016%
92	15.168	4312	4316	4321	rBV3	881	978	0.18%	0.018%
93	15.219	4322	4332	4353	rVB	108847	179953	32.51%	3.223%
94	15.406	4379	4390	4404	rBV	72811	121978	22.04%	2.185%
95	15.544	4430	4433	4440	rVB4	483	454	0.08%	0.008%
96	15.820	4514	4519	4522	rBV2	699	671	0.12%	0.012%
97	15.952	4553	4560	4571	rBV3	4580	7097	1.28%	0.127%
98	16.123	4611	4613	4616	rBV	576	326	0.06%	0.006%
99	16.264	4649	4657	4667	rBV5	6434	10698	1.93%	0.192%
100	16.406	4694	4701	4709	rBV4	9755	15582	2.82%	0.279%

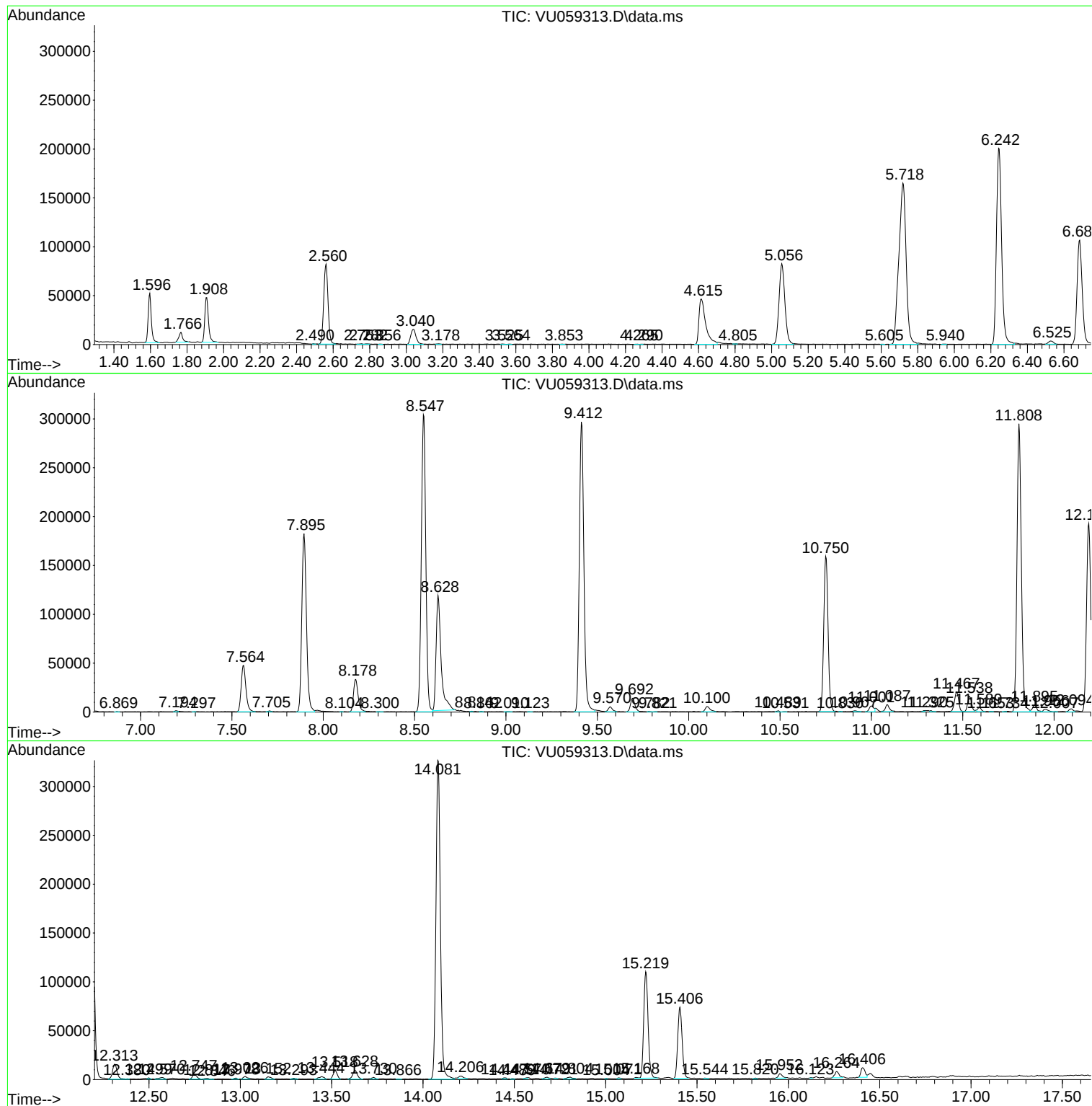
Sum of corrected areas: 5583556

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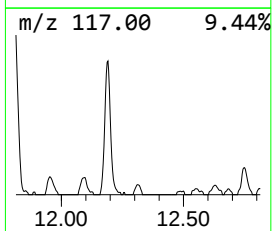
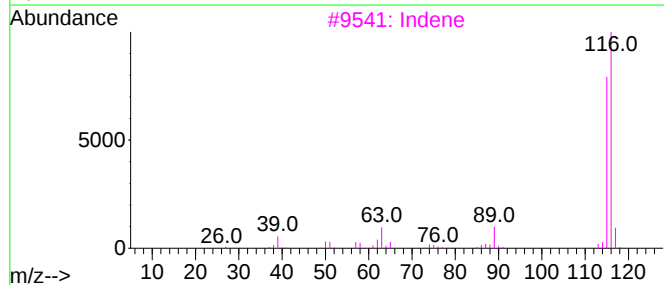
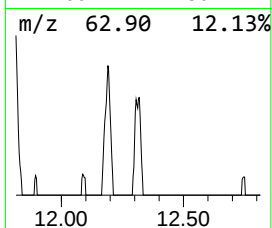
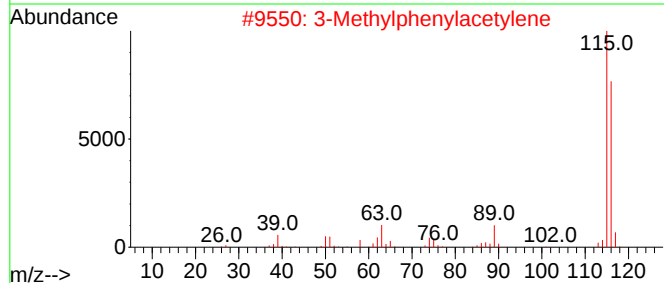
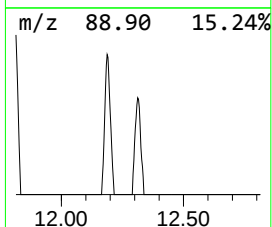
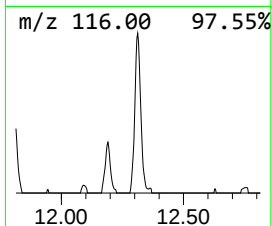
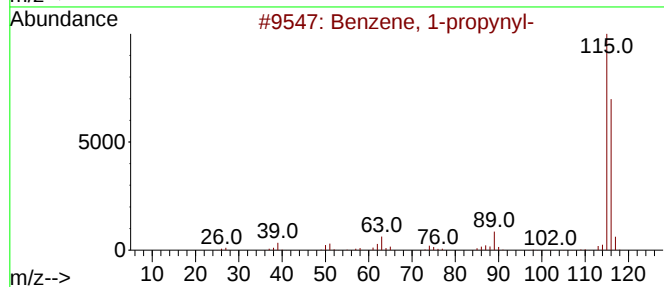
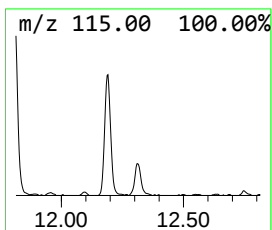
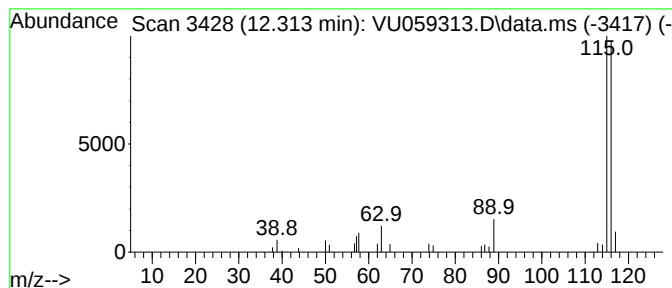
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Benzene, 1-propynyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.313	2.75 ug/L	26554	1,4-Dichlorobenzene-d4	11.808

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
2			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
3			Indene	116	C9H8	000095-13-6	91
4			Indene	116	C9H8	000095-13-6	91
5			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	90



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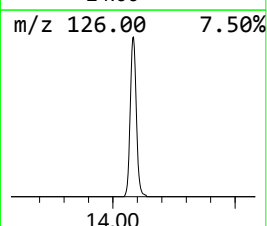
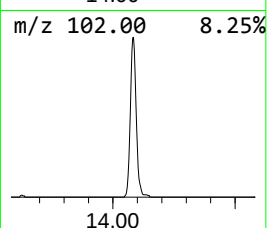
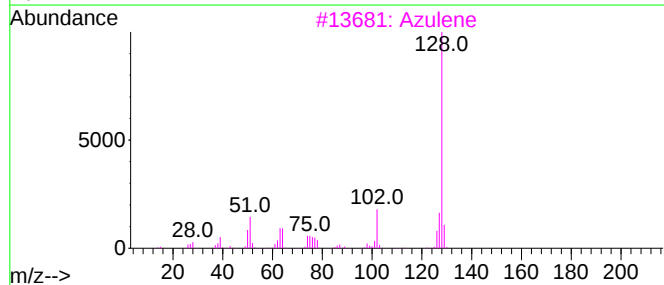
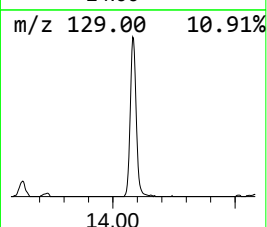
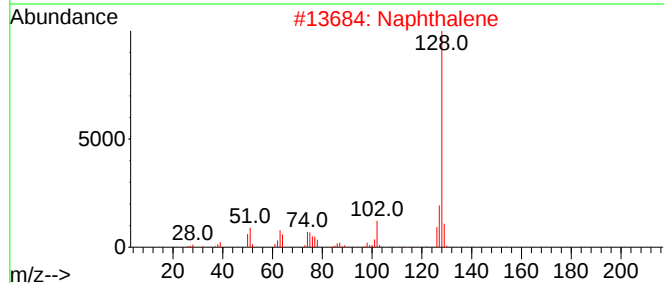
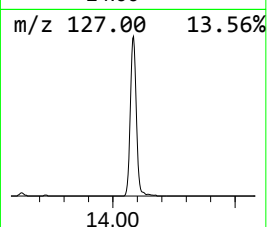
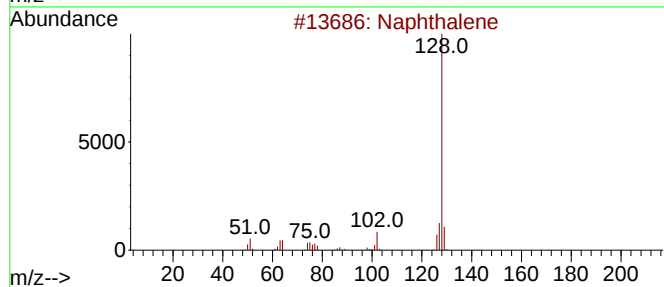
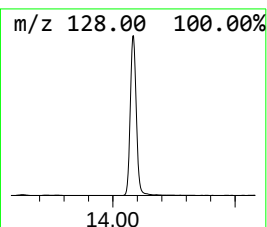
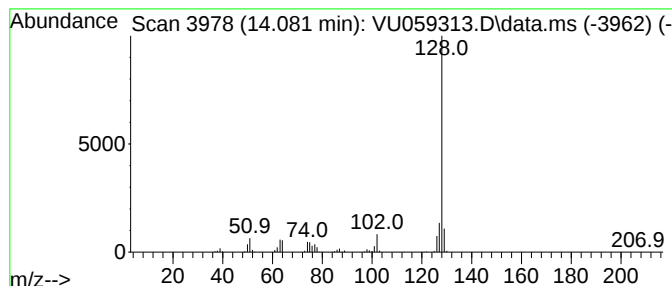
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.081	57.22 ug/L	553500	1,4-Dichlorobenzene-d4	11.808

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, 1-prop...	12.313	2.8	ug/L	26554	3	11.808	483654	50.0
Azulene	14.081	57.2	ug/L	553500	3	11.808	483654	50.0