

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
 Data File : VU045251.D
 Acq On : 08 Oct 2021 15:05
 Operator : SY/MD
 Sample : M4024-15DL 5X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AM3DL

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\SFAMULM092321WMA.M

Title : VOC Analysis

Signal : TIC: VU045251.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.475	33	42	54	rBV	123291	259957	19.49%	2.210%
2	1.601	75	81	96	rVB2	419125	486487	36.47%	4.136%
3	1.893	166	172	194	rVB	149792	228121	17.10%	1.940%
4	2.562	368	380	398	rBV	276138	464238	34.81%	3.947%
5	2.684	410	418	429	rVB2	6862	12424	0.93%	0.106%
6	2.797	442	453	459	rBV2	3659	7385	0.55%	0.063%
7	3.047	524	531	544	rVB2	5538	9659	0.72%	0.082%
8	3.346	622	624	633	rVB5	1192	1569	0.12%	0.013%
9	3.504	670	673	676	rBV	322	250	0.02%	0.002%
10	3.874	772	788	807	rVB	15879	35762	2.68%	0.304%
11	4.141	866	871	874	rBV	284	220	0.02%	0.002%
12	4.565	997	1003	1005	rBV3	952	940	0.07%	0.008%
13	4.629	1009	1023	1029	rBV	144179	317384	23.80%	2.698%
14	4.928	1114	1116	1122	rVB2	282	219	0.02%	0.002%
15	5.067	1143	1159	1180	rBV	231866	505686	37.91%	4.299%
16	5.202	1197	1201	1204	rBV2	336	315	0.02%	0.003%
17	5.292	1223	1229	1232	rBV3	725	919	0.07%	0.008%
18	5.314	1232	1236	1244	rVB4	859	1134	0.09%	0.010%
19	5.584	1318	1320	1326	rVB2	252	238	0.02%	0.002%
20	5.729	1336	1365	1393	rBV2	495866	1333812	100.00%	11.340%
21	5.848	1400	1402	1406	rVB3	464	252	0.02%	0.002%
22	5.896	1414	1417	1422	rBV3	343	372	0.03%	0.003%
23	5.973	1438	1441	1443	rBV2	382	213	0.02%	0.002%
24	6.131	1486	1490	1494	rVB3	558	469	0.04%	0.004%
25	6.169	1500	1502	1509	rVB	372	214	0.02%	0.002%
26	6.253	1513	1528	1548	rBV	356961	673456	50.49%	5.726%
27	6.510	1595	1608	1618	rBV3	9861	22855	1.71%	0.194%
28	6.694	1651	1665	1684	rBV	310776	602899	45.20%	5.126%
29	6.806	1693	1700	1716	rVB4	5557	10775	0.81%	0.092%
30	6.970	1739	1751	1764	rBV3	4368	8712	0.65%	0.074%
31	7.044	1769	1774	1783	rVB2	572	853	0.06%	0.007%
32	7.182	1810	1817	1826	rVB3	1168	1674	0.13%	0.014%
33	7.247	1831	1837	1842	rBV3	468	652	0.05%	0.006%
34	7.568	1924	1937	1957	rBV	170280	293450	22.00%	2.495%
35	7.687	1970	1974	1983	rVB4	744	1088	0.08%	0.009%
36	7.903	2026	2041	2054	rBV	604117	1022684	76.67%	8.695%

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 Title : VOC Analysis

37	7.973	2054	2063	2078	rVB	31134	53673	4.02%	0.456%
38	8.031	2078	2081	2084	rBV2	386	324	0.02%	0.003%
39	8.182	2115	2128	2143	rBV	120493	196604	14.74%	1.672%
40	8.378	2186	2189	2192	rBV	405	304	0.02%	0.003%
41	8.484	2219	2222	2232	rVB3	1255	1950	0.15%	0.017%
42	8.636	2256	2269	2311	rBV	418728	735679	55.16%	6.255%
43	8.784	2313	2315	2325	rVV6	1082	1242	0.09%	0.011%
44	8.947	2362	2366	2369	rBV2	259	281	0.02%	0.002%
45	9.044	2391	2396	2399	rBV2	776	677	0.05%	0.006%
46	9.420	2499	2513	2531	rBV	523706	847169	63.51%	7.203%
47	9.574	2549	2561	2574	rBV	142034	226844	17.01%	1.929%
48	9.693	2585	2598	2612	rBV	373377	602367	45.16%	5.121%
49	9.970	2681	2684	2692	rVB2	266	314	0.02%	0.003%
50	10.105	2714	2726	2745	rBV	86494	139517	10.46%	1.186%
51	10.320	2786	2793	2797	rVB2	219	228	0.02%	0.002%
52	10.488	2835	2845	2856	rVB2	19058	28125	2.11%	0.239%
53	10.671	2894	2902	2911	rVV2	4401	6582	0.49%	0.056%
54	10.761	2917	2930	2949	rBV	432970	696001	52.18%	5.918%
55	10.835	2949	2953	2959	rVB3	339	361	0.03%	0.003%
56	10.867	2959	2963	2967	rBV2	859	972	0.07%	0.008%
57	10.925	2968	2981	2993	rVB4	9312	21298	1.60%	0.181%
58	10.992	2996	3002	3011	rBV5	2278	3604	0.27%	0.031%
59	11.092	3025	3033	3033	rBV3	735	1045	0.08%	0.009%
60	11.153	3049	3052	3057	rVB2	383	333	0.02%	0.003%
61	11.298	3090	3097	3105	rVV2	1074	1428	0.11%	0.012%
62	11.359	3113	3116	3121	rVB	312	278	0.02%	0.002%
63	11.472	3139	3151	3164	rVB4	9329	16802	1.26%	0.143%
64	11.581	3180	3185	3188	rBV2	675	590	0.04%	0.005%
65	11.700	3213	3222	3229	rBV3	1984	2936	0.22%	0.025%
66	11.816	3240	3258	3272	rBV	496208	813148	60.96%	6.914%
67	11.944	3292	3298	3301	rBV4	1003	1212	0.09%	0.010%
68	11.976	3304	3308	3315	rVB4	3073	3749	0.28%	0.032%
69	12.012	3315	3319	3322	rBV2	546	547	0.04%	0.005%
70	12.063	3332	3335	3338	rVV2	1028	757	0.06%	0.006%
71	12.098	3338	3346	3359	rVB	9559	14906	1.12%	0.127%
72	12.195	3359	3376	3397	rBV	538142	876332	65.70%	7.451%
73	12.304	3405	3410	3411	rBV4	1217	892	0.07%	0.008%
74	12.378	3428	3433	3434	rBV	573	441	0.03%	0.004%
75	12.574	3488	3494	3498	rBV2	508	558	0.04%	0.005%
76	12.642	3512	3515	3522	rVB3	655	586	0.04%	0.005%

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 Title : VOC Analysis

77	12.687	3522	3529	3537	rBV3	2165	2923	0.22%	0.025%
78	12.774	3551	3556	3558	rBV	334	276	0.02%	0.002%
79	12.809	3563	3567	3571	rBV2	250	235	0.02%	0.002%
80	12.841	3572	3577	3580	rBV3	301	259	0.02%	0.002%
81	12.867	3582	3585	3593	rVB3	549	641	0.05%	0.005%
82	12.954	3603	3612	3618	rBV3	5958	9901	0.74%	0.084%
83	13.037	3633	3638	3645	rBV3	853	955	0.07%	0.008%
84	13.108	3657	3660	3662	rBV2	326	236	0.02%	0.002%
85	13.250	3700	3704	3707	rBV2	348	387	0.03%	0.003%
86	13.459	3766	3769	3778	rVB4	1003	1011	0.08%	0.009%
87	13.709	3842	3847	3851	rVB2	210	224	0.02%	0.002%
88	13.745	3851	3858	3865	rBV4	2159	2952	0.22%	0.025%
89	13.790	3865	3872	3879	rVV3	490	805	0.06%	0.007%
90	13.883	3896	3901	3903	rBV2	502	465	0.03%	0.004%
91	14.092	3954	3966	3981	rBV	71797	116434	8.73%	0.990%
92	14.208	3992	4002	4013	rVB4	3547	6722	0.50%	0.057%
93	14.291	4020	4028	4034	rBV3	2923	3885	0.29%	0.033%
94	14.359	4047	4049	4053	rVB	506	326	0.02%	0.003%
95	14.385	4053	4057	4061	rBV3	379	392	0.03%	0.003%
96	14.426	4064	4070	4073	rBV3	440	518	0.04%	0.004%
97	14.671	4142	4146	4148	rBV3	447	381	0.03%	0.003%
98	14.925	4221	4225	4228	rBV2	348	311	0.02%	0.003%
99	15.420	4370	4379	4388	rBV3	1723	3102	0.23%	0.026%
100	16.491	4710	4712	4715	rBV3	440	293	0.02%	0.002%

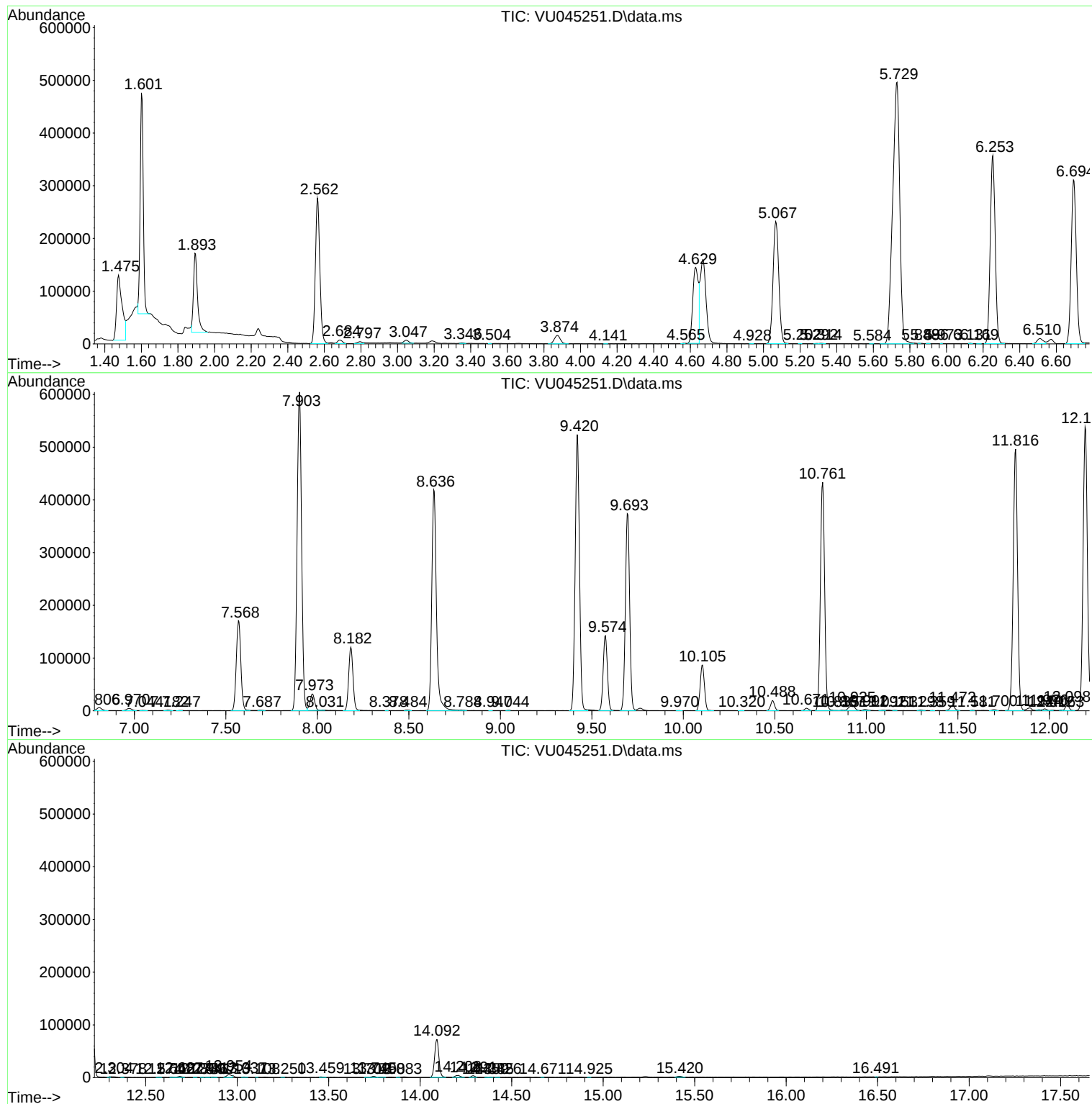
Sum of corrected areas: 11761627

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.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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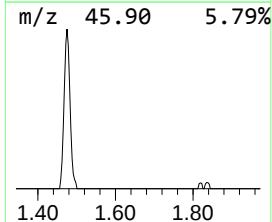
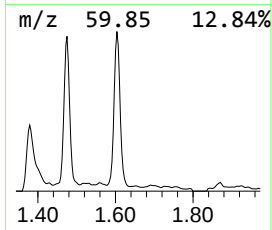
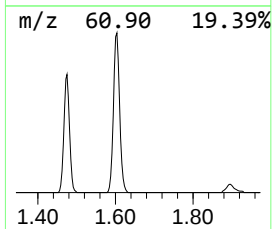
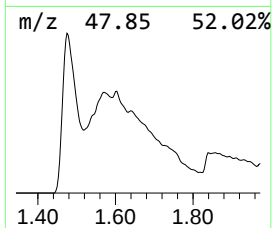
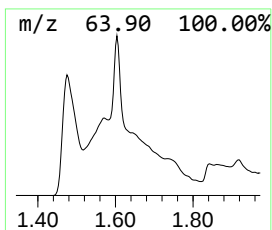
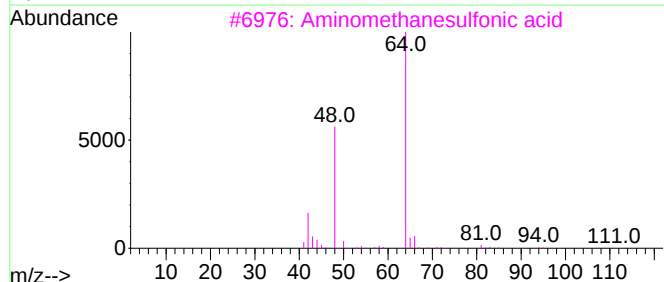
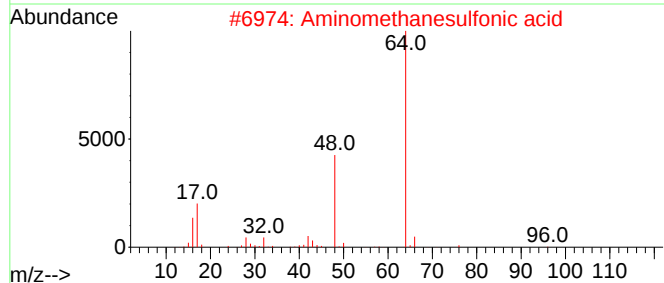
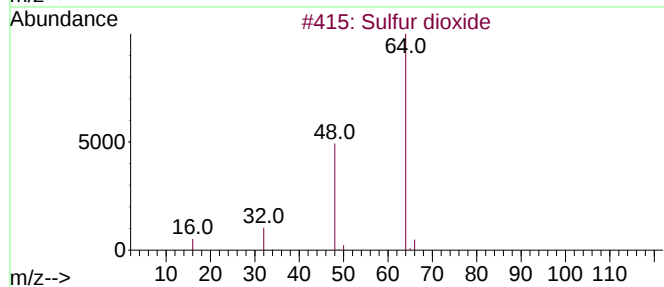
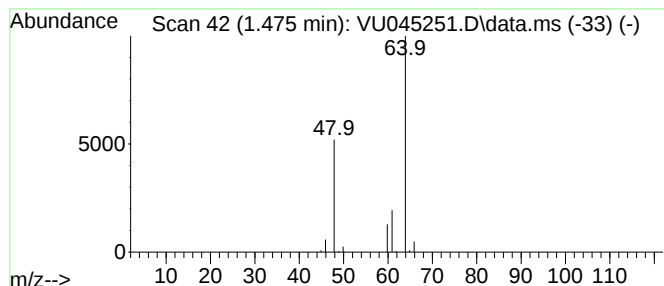
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.475	19.30 ug/L	259957	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	78
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	5



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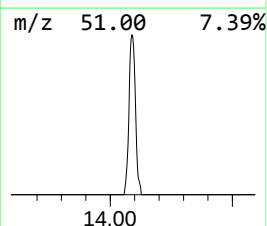
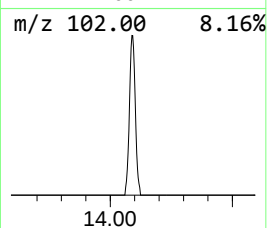
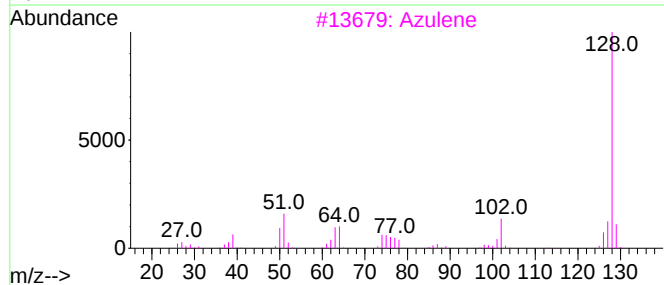
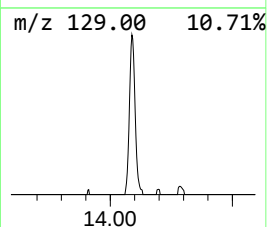
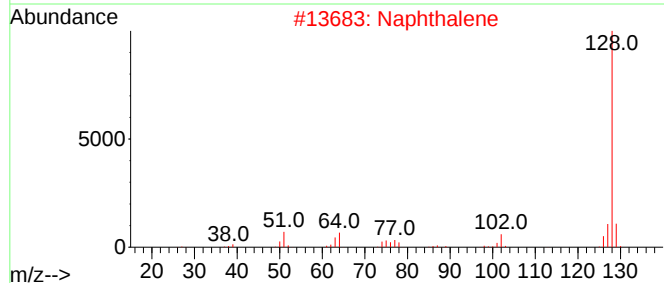
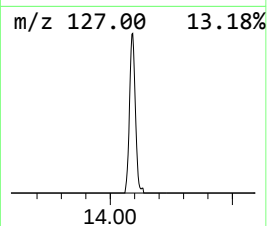
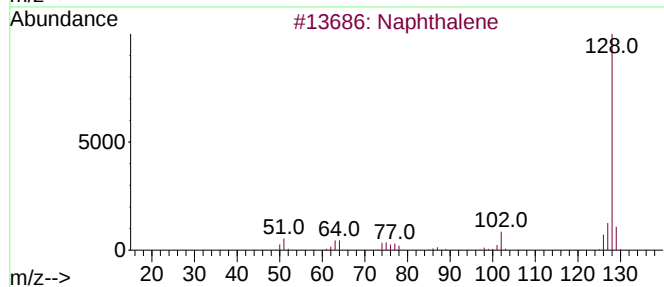
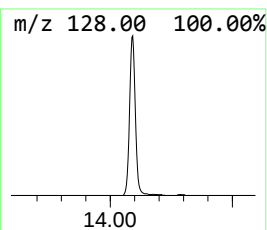
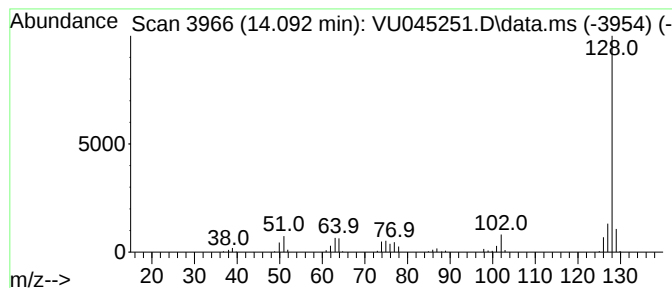
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Quant Title : VOC Analysis

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.
14.092	7.16 ug/L	116434	1,4-Dichlorobenzene-d4	11.816

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			Naphthalene	128	C10H8	000091-20-3	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.475	19.3	ug/L	259957	1	6.253	673456	50.0
Azulene	14.092	7.2	ug/L	116434	3	11.816	813148	50.0