

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU073124\
 Data File : VU060281.D
 Acq On : 31 Jul 2024 14:01
 Operator : MD/SY
 Sample : P3287-05
 Misc : 10.00g/10.0mL//100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 XB504

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\SFAMULM070224WMA.M

Title : VOC Analysis

Signal : TIC: VU060281.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.592	87	94	120	rVB	56076	100202	2.50%	0.229%
2	1.850	138	174	176	rBV4	39232	135430	3.38%	0.309%
3	2.538	375	388	406	rBV	111224	210823	5.26%	0.481%
4	2.634	407	418	453	rVB	193955	523333	13.06%	1.194%
5	2.901	494	501	502	rBV5	1076	1098	0.03%	0.003%
6	2.949	507	516	526	rBV	14969	28657	0.72%	0.065%
7	3.026	527	540	583	rVV	462411	1196132	29.85%	2.730%
8	3.361	626	644	672	rVV	197120	471504	11.77%	1.076%
9	3.525	692	695	698	rBV2	397	291	0.01%	0.001%
10	3.637	727	730	733	rBV	229	236	0.01%	0.001%
11	3.670	734	740	744	rVV3	927	1339	0.03%	0.003%
12	3.933	818	822	829	rVB	300	355	0.01%	0.001%
13	4.174	891	897	901	rBV2	248	314	0.01%	0.001%
14	4.496	989	997	1001	rVB2	356	569	0.01%	0.001%
15	4.650	1026	1045	1053	rBV2	367291	898881	22.43%	2.051%
16	5.071	1156	1176	1198	rBV4	211317	636762	15.89%	1.453%
17	5.329	1251	1256	1259	rBV2	373	375	0.01%	0.001%
18	5.711	1356	1375	1386	rBV2	244635	625385	15.61%	1.427%
19	5.782	1387	1397	1423	rVB	525880	1081396	26.99%	2.468%
20	6.097	1490	1495	1498	rBV3	451	418	0.01%	0.001%
21	6.177	1518	1520	1527	rVB2	388	383	0.01%	0.001%
22	6.239	1527	1539	1569	rBV	282340	560218	13.98%	1.278%
23	6.444	1599	1603	1606	rBV2	282	230	0.01%	0.001%
24	6.528	1621	1629	1641	rVV10	2853	5763	0.14%	0.013%
25	6.634	1657	1662	1664	rBV2	230	260	0.01%	0.001%
26	6.682	1664	1677	1694	rBV	141578	281578	7.03%	0.643%
27	6.782	1694	1708	1734	rVB	487182	948982	23.68%	2.166%
28	6.907	1734	1747	1772	rBV	601923	1169357	29.18%	2.669%
29	7.097	1793	1806	1829	rBV	186875	365266	9.12%	0.834%
30	7.213	1829	1842	1868	rBV2	45363	93579	2.34%	0.214%
31	7.390	1894	1897	1902	rVB2	586	409	0.01%	0.001%
32	7.447	1907	1915	1921	rBV4	953	1592	0.04%	0.004%
33	7.560	1939	1950	1953	rBV	80336	117724	2.94%	0.269%
34	7.599	1954	1962	1989	rVV	608226	1111023	27.73%	2.535%
35	7.718	1991	1999	2021	rVB2	16171	33801	0.84%	0.077%
36	7.891	2041	2053	2064	rBV	286846	509917	12.73%	1.164%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.M
 Title : VOC Analysis

37	7.962	2064	2075	2108	rVB	2017440	3490928	87.12%	7.966%
38	8.203	2131	2150	2174	rBV2	257242	571379	14.26%	1.304%
39	8.306	2180	2182	2186	rVB2	626	453	0.01%	0.001%
40	8.335	2186	2191	2194	rBV5	597	474	0.01%	0.001%
41	8.402	2208	2212	2216	rBV3	1807	2092	0.05%	0.005%
42	8.547	2243	2257	2274	rVV	517518	881682	22.00%	2.012%
43	8.640	2274	2286	2290	rVV2	157432	282556	7.05%	0.645%
44	8.689	2291	2301	2327	rVV	1262272	2595797	64.78%	5.924%
45	8.804	2328	2337	2354	rVB	83951	168660	4.21%	0.385%
46	8.917	2360	2372	2392	rVB	263008	473903	11.83%	1.081%
47	9.081	2420	2423	2427	rBV3	319	301	0.01%	0.001%
48	9.103	2428	2430	2435	rVB3	518	272	0.01%	0.001%
49	9.136	2435	2440	2442	rVB4	297	264	0.01%	0.001%
50	9.171	2447	2451	2452	rBV2	334	223	0.01%	0.001%
51	9.206	2458	2462	2463	rBV2	426	327	0.01%	0.001%
52	9.232	2467	2470	2474	rVB2	401	325	0.01%	0.001%
53	9.354	2504	2508	2512	rBV2	279	279	0.01%	0.001%
54	9.441	2513	2535	2550	rBV2	1022243	2494387	62.25%	5.692%
55	9.531	2550	2563	2569	rBV	985603	1782055	44.48%	4.067%
56	9.689	2599	2612	2645	rVB	1141224	1971314	49.20%	4.499%
57	9.943	2686	2691	2694	rVB2	359	305	0.01%	0.001%
58	9.959	2694	2696	2702	rBV2	308	269	0.01%	0.001%
59	10.033	2716	2719	2720	rBV2	376	224	0.01%	0.001%
60	10.110	2727	2743	2784	rBV2	2196598	4006855	100.00%	9.144%
61	10.290	2786	2799	2821	rVB	203894	371869	9.28%	0.849%
62	10.370	2821	2824	2826	rBV2	594	454	0.01%	0.001%
63	10.412	2834	2837	2840	rVB2	466	312	0.01%	0.001%
64	10.476	2852	2857	2860	rBV4	2099	2160	0.05%	0.005%
65	10.589	2889	2892	2897	rVB3	294	289	0.01%	0.001%
66	10.615	2897	2900	2902	rBV	301	235	0.01%	0.001%
67	10.753	2931	2943	2953	rBV	231989	375468	9.37%	0.857%
68	10.820	2953	2964	2990	rVB	1307133	2171978	54.21%	4.957%
69	10.949	3002	3004	3009	rVB3	353	231	0.01%	0.001%
70	10.975	3009	3012	3016	rBV2	431	284	0.01%	0.001%
71	11.016	3023	3025	3027	rBV2	810	510	0.01%	0.001%
72	11.094	3043	3049	3054	rBV4	1009	1149	0.03%	0.003%
73	11.123	3056	3058	3065	rVV2	461	468	0.01%	0.001%
74	11.164	3069	3071	3076	rVB	450	312	0.01%	0.001%
75	11.377	3133	3137	3138	rBV	557	400	0.01%	0.001%
76	11.425	3147	3152	3153	rBV2	961	665	0.02%	0.002%

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77	11.473	3159	3167	3171	rBV4	1608	1894	0.05%	0.004%
78	11.512	3177	3179	3185	rVB4	796	582	0.01%	0.001%
79	11.563	3190	3195	3200	rBV2	445	448	0.01%	0.001%
80	11.595	3200	3205	3206	rBV	251	221	0.01%	0.001%
81	11.743	3238	3251	3262	rBV	1013649	1613013	40.26%	3.681%
82	11.830	3262	3278	3298	rVB2	1111745	2484409	62.00%	5.670%
83	11.978	3321	3324	3329	rVB3	639	599	0.01%	0.001%
84	12.000	3329	3331	3334	rVB	591	279	0.01%	0.001%
85	12.029	3334	3340	3344	rBV3	612	639	0.02%	0.001%
86	12.206	3377	3395	3424	rBV2	1544315	2858255	71.33%	6.523%
87	12.370	3443	3446	3448	rVB2	606	295	0.01%	0.001%
88	12.473	3469	3478	3487	rVB4	9703	14498	0.36%	0.033%
89	12.991	3626	3639	3662	rBV	356221	577779	14.42%	1.319%
90	13.229	3710	3713	3717	rVB2	396	295	0.01%	0.001%
91	13.389	3758	3763	3764	rBV2	450	394	0.01%	0.001%
92	13.483	3788	3792	3795	rBV2	424	420	0.01%	0.001%
93	13.566	3816	3818	3824	rBV2	333	337	0.01%	0.001%
94	13.650	3840	3844	3847	rBV3	386	290	0.01%	0.001%
95	13.772	3878	3882	3884	rBV	276	258	0.01%	0.001%
96	13.814	3887	3895	3900	rBV3	6023	8764	0.22%	0.020%
97	14.016	3945	3958	3968	rBV	991130	1544068	38.54%	3.524%
98	14.081	3968	3978	4008	rVB	1240789	1945380	48.55%	4.439%
99	14.328	4051	4055	4060	rVB4	1094	1011	0.03%	0.002%
100	14.598	4136	4139	4142	rBV2	578	382	0.01%	0.001%

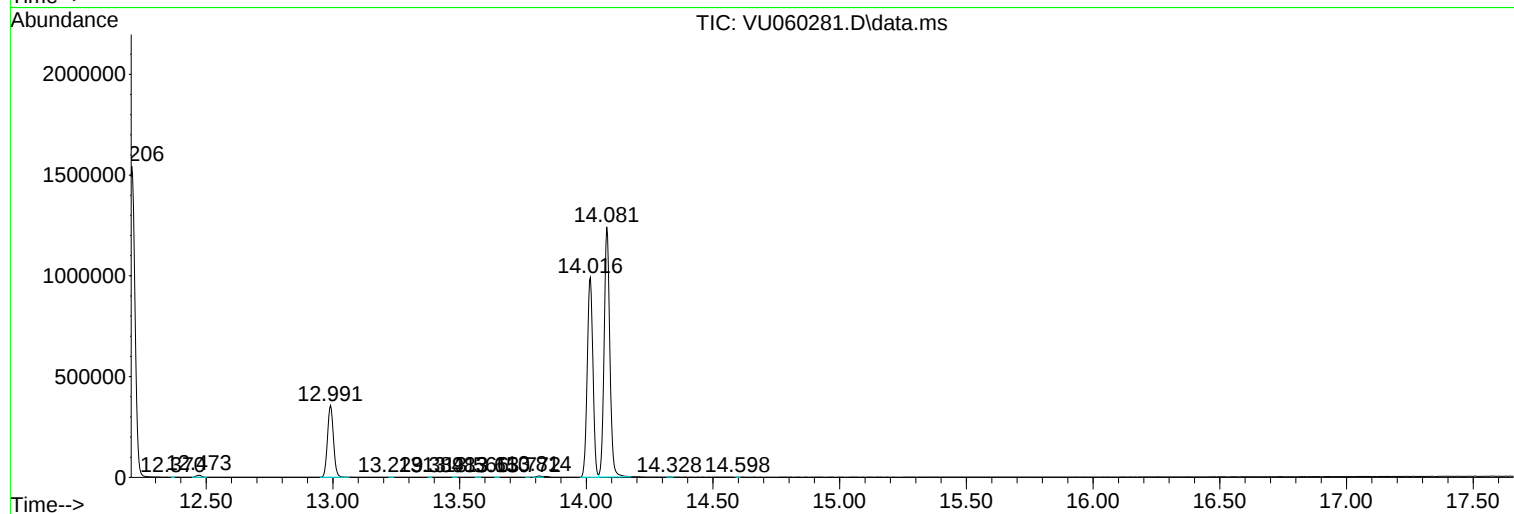
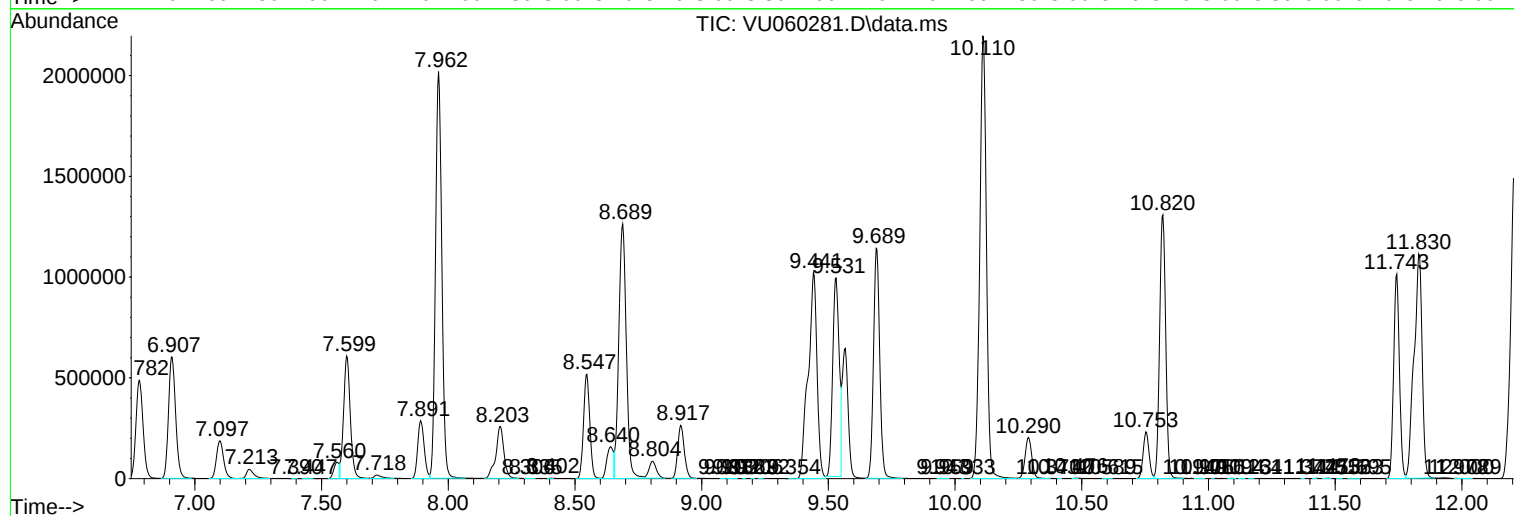
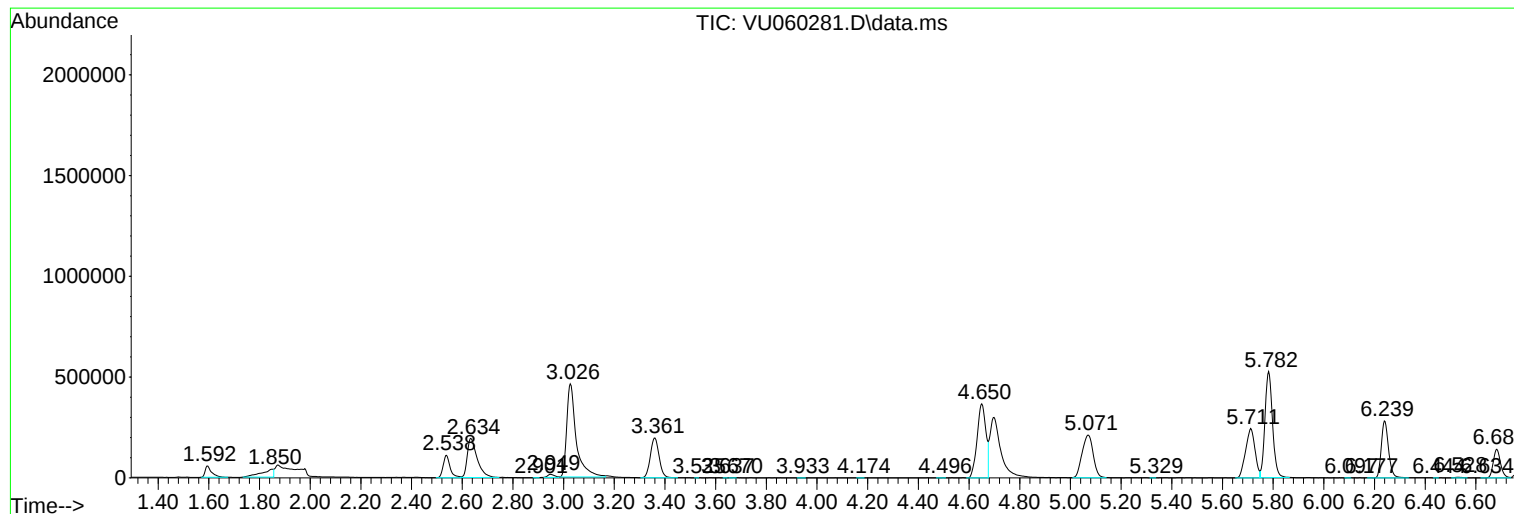
Sum of corrected areas: 43820200

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.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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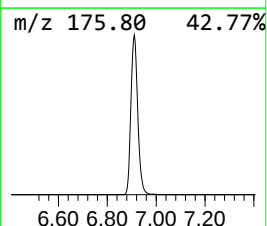
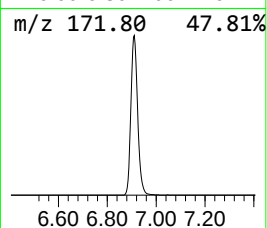
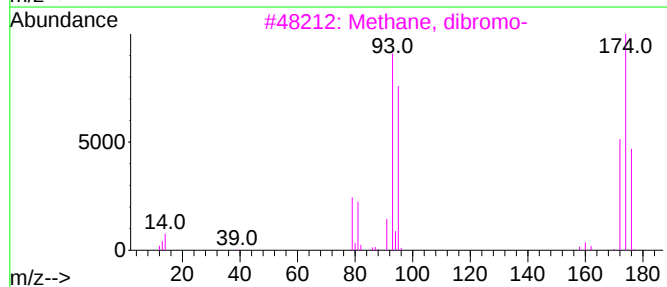
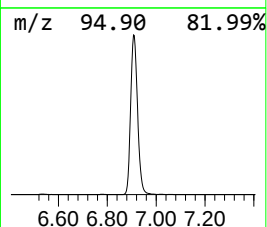
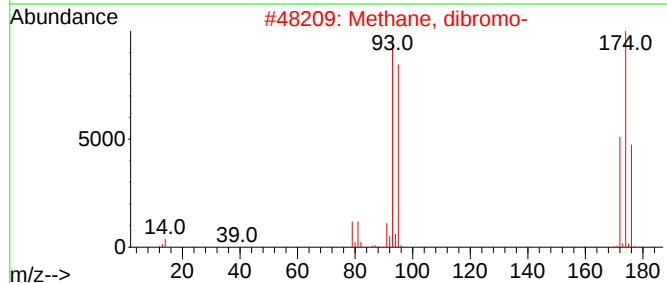
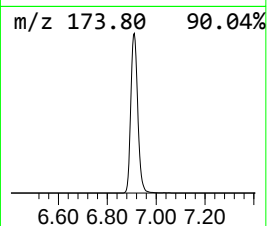
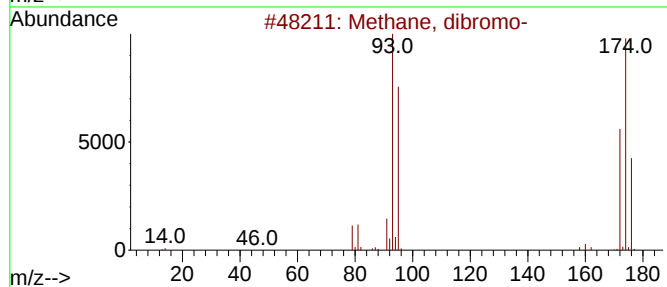
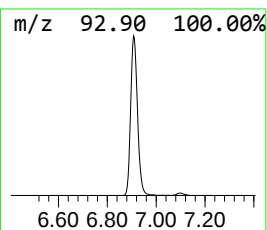
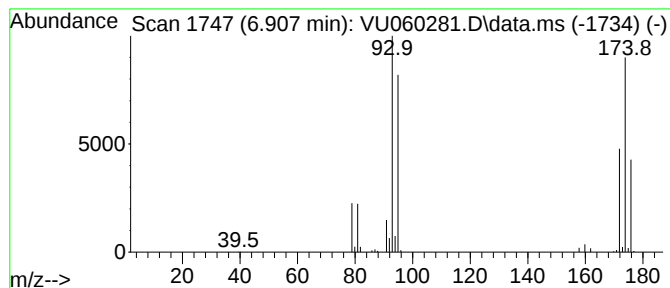
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Methane, dibromo- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.907	104.37 ug/L	1169360	1,4-Difluorobenzene	6.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methane, dibromo-	172	CH2Br2	000074-95-3	96
2			Methane, dibromo-	172	CH2Br2	000074-95-3	96
3			Methane, dibromo-	172	CH2Br2	000074-95-3	94
4			Methane, dibromo-	172	CH2Br2	000074-95-3	91
5			Dimethyl selenodisulfide	174	C2H6S2Se	1000357-25-9	9



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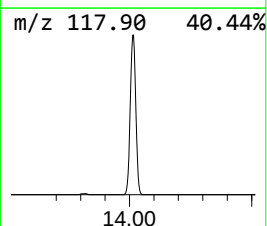
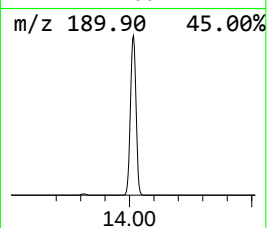
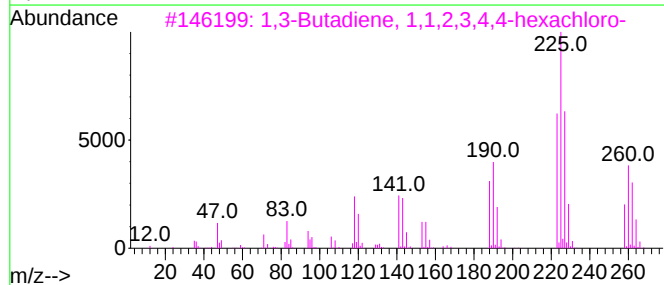
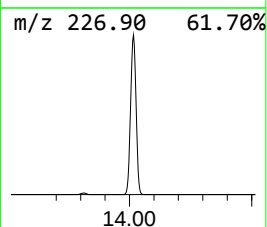
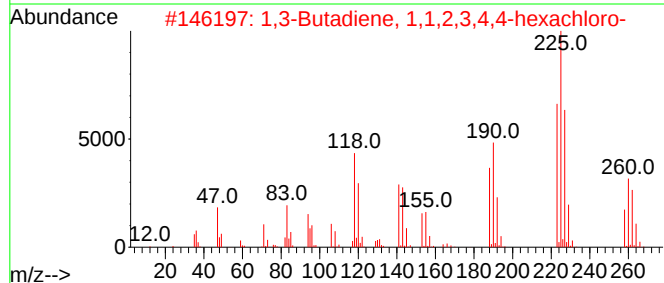
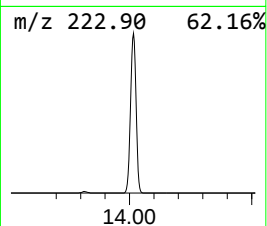
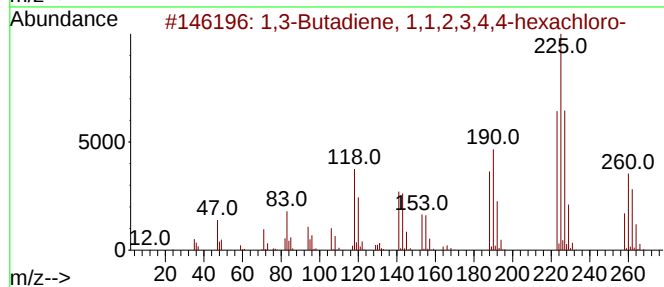
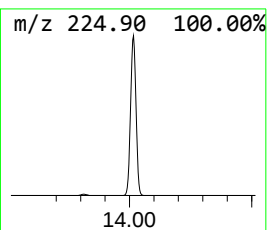
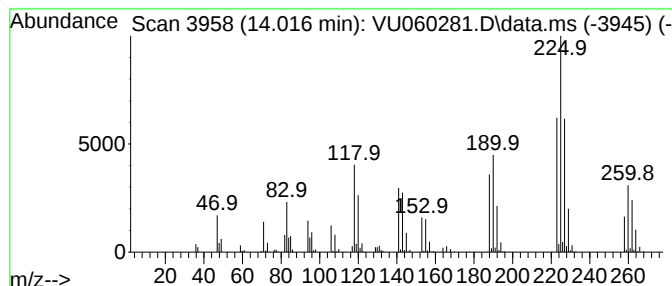
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 1,3-Butadiene, 1,1,2,3,4,4-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.016	31.08 ug/L	1544070	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	99
2			1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	99
3			1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	99
4			1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	99
5			5H-dibenzo[a,d]cycloheptene, 5,1...	260	C15H10Cl2	1000401-56-4	17



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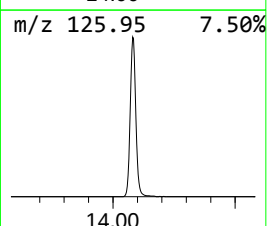
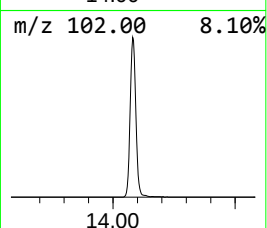
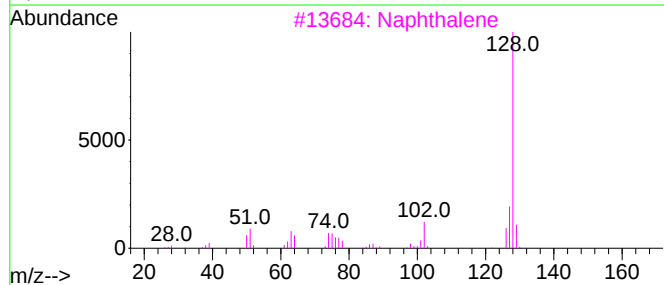
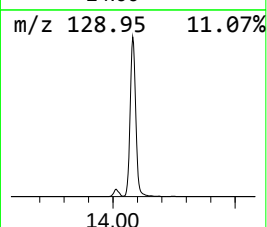
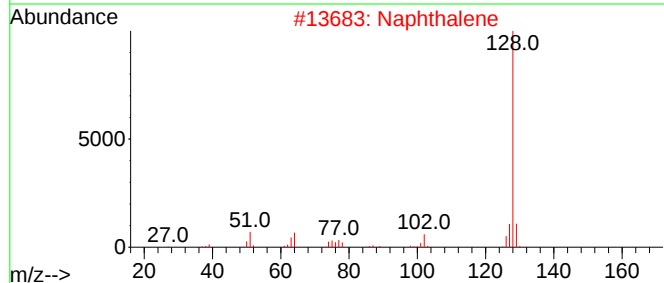
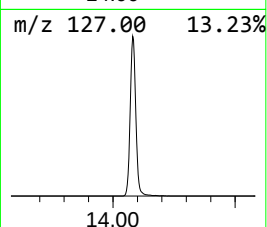
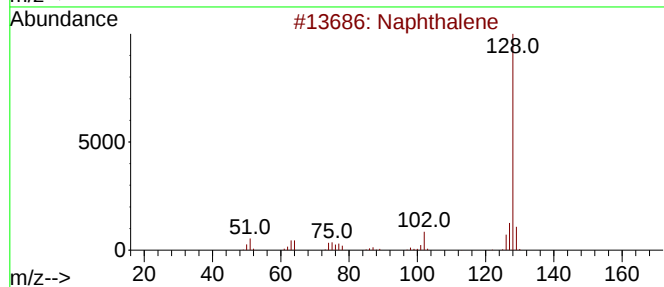
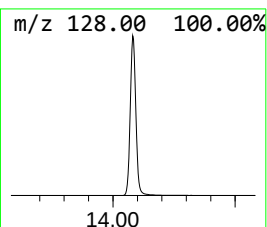
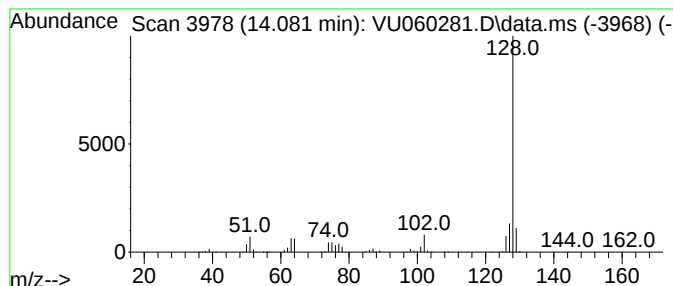
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 Azulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.081	39.15 ug/L	1945380	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			Naphthalene	128	C10H8	000091-20-3	94
4			Azulene	128	C10H8	000275-51-4	91
5			Azulene	128	C10H8	000275-51-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU073124\
Data File : VU060281.D
Acq On : 31 Jul 2024 14:01
Operator : MD/SY
Sample : P3287-05
Misc : 10.00g/10.0mL//100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
XB504

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Methane, dibromo-	6.907	104.4	ug/L	1169360	1	6.239	560218	50.0
1,3-Butadiene, ...	14.016	31.1	ug/L	1544070	3	11.807	2484410	50.0
Azulene	14.081	39.1	ug/L	1945380	3	11.807	2484410	50.0