LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU073124\
Data File : VU060283.D
Acq On : 31 Jul 2024 14:52
Operator : MD/SY
Sample : P3287-05DL 5X
Misc : 10.00g/10.0mL//100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
XB504DL

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: VU060283.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	rBV	99398	124017	13.05%	1.009%
2	1.824	140	166	171	rBV4	21621	63582	6.69%	0.517%
3	1.888	178	186	201	rVB	65824	98382	10.35%	0.800%
4	2.554	381	393	404	rBV	152026	248258	26.12%	2.020%
5	2.618	405	413	432	rVB	53735	95961	10.10%	0.781%
6	2.776	459	462	465	rBV3	408	318	0.03%	0.003%
7	2.949	508	516	526	rBV2	2653	4624	0.49%	0.038%
8	3.033	529	542	573	rBV2	116400	251044	26.41%	2.042%
9	3.351	626	641	659	rBV	36926	85699	9.02%	0.697%
10	3.631	725	728	734	rBV2	216	211	0.02%	0.002%
11	3.776	768	773	777	rBV2	228	220	0.02%	0.002%
12	3.850	793	796	802	rVB2	333	316	0.03%	0.003%
13	3.898	802	811	815	rBV2	329	493	0.05%	0.004%
14	4.036	846	854	858	rVB	302	379	0.04%	0.003%
15	4.139	882	886	890	rVB2	288	256	0.03%	0.002%
16	4.258	920	923	926	rVB2	346	213	0.02%	0.002%
17	4.280	926	930	934	rBV	204	242	0.03%	0.002%
18	4.483	986	993	999	rBV2	254	291	0.03%	0.002%
19	4.615	1024	1034	1039	rBV	68130	125363	13.19%	1.020%
20	5.055	1155	1171	1201	rBV3	134280	356931	37.55%	2.904%
21	5.399	1274	1278	1281	rVB2	228	214	0.02%	0.002%
22	5.428	1282	1287	1288	rBV2	329	235	0.02%	0.002%
23	5.605	1336	1342	1346	rBV	357	349	0.04%	0.003%
24	5.714	1356	1376	1389	rBV2	268285	717468	75.48%	5.837%
25	5.785	1390	1398	1420	rVB	106042	214429	22.56%	1.744%
26	5.888	1427	1430	1435	rVB3	433	332	0.03%	0.003%
27	5.917	1435	1439	1443	rBV2	370	289	0.03%	0.002%
28	6.242	1527	1540	1571	rBV	277186	537177	56.51%	4.370%
29	6.422	1595	1596	1603	rVV3	254	220	0.02%	0.002%
30	6.528	1620	1629	1639	rVB6	2620	5258	0.55%	0.043%
31	6.576	1640	1644	1648	rBV3	314	295	0.03%	0.002%
32	6.624	1653	1659	1661	rBV2	264	290	0.03%	0.002%
33	6.682	1665	1677	1696	rBV	167183	324469	34.14%	2.640%
34	6.782	1696	1708	1731	rVB	96013	185902	19.56%	1.512%
35	6.911	1736	1748	1770	rBV2	119005	227112	23.89%	1.848%
36	7.100	1793	1807	1823	rVV2	37623	70327	7.40%	0.572%

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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
XB504DL

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

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Peak separation: 5

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

37	7.219	1837	1844	1860	rVV2	6519	12576	1.32%	0.102%
38	7.322	1872	1876	1882	rBV2	306	307	0.03%	0.002%
39	7.351	1882	1885	1890	rVV2	246	237	0.02%	0.002%
40	7.383	1890	1895	1901	rVV2	320	345	0.04%	0.003%
41	7.486	1922	1927	1929	rBV2	242	219	0.02%	0.002%
42	7.560	1933	1950	1956	rBV2	87519	150099	15.79%	1.221%
43	7.602	1957	1963	1984	rVB	109501	192819	20.29%	1.569%
44	7.730	1994	2003	2013	rBV5	2325	4767	0.50%	0.039%
45	7.891	2041	2053	2065	rBV	319419	549541	57.81%	4.471%
46	7.962	2065	2075	2098	rVB	371852	643892	67.74%	5.238%
47	8.174	2131	2141	2147	rBV	64071	111669	11.75%	0.908%
48	8.274	2170	2172	2178	rVB3	689	635	0.07%	0.005%
49	8.402	2210	2212	2215	rVV2	457	273	0.03%	0.002%
50	8.547	2245	2257	2272	rBV	105343	175658	18.48%	1.429%
51	8.628	2272	2282	2290	rVV	183654	319291	33.59%	2.598%
52	8.679	2291	2298	2327	rVV	269969	483367	50.85%	3.932%
53	8.804	2329	2337	2351	rVB2	17823	31627	3.33%	0.257%
54	8.917	2360	2372	2387	rBV	50752	88196	9.28%	0.717%
55	9.071	2416	2420	2423	rBV2	276	271	0.03%	0.002%
56	9.139	2437	2441	2445	rVB2	296	293	0.03%	0.002%
57	9.161	2445	2448	2450	rBV	278	214	0.02%	0.002%
58	9.412	2513	2526	2533	rBV	431030	769790	80.98%	6.262%
59	9.528	2551	2562	2569	rBV	196546	331907	34.92%	2.700%
60	9.689	2599	2612	2636	rBV	192923	332563	34.99%	2.705%
61	9.881	2670	2672	2675	rVB3	390	234	0.02%	0.002%
62	9.914	2675	2682	2686	rBV2	338	484	0.05%	0.004%
63	10.110	2728	2743	2780	rVV2	329107	620272	65.26%	5.046%
64	10.283	2786	2797	2812	rVV2	37024	63936	6.73%	0.520%
65	10.344	2812	2816	2819	rVB2	725	626	0.07%	0.005%
66	10.370	2819	2824	2827	rBV	325	284	0.03%	0.002%
67	10.444	2844	2847	2853	rBV2	224	263	0.03%	0.002%
68	10.473	2853	2856	2859	rBV	205	209	0.02%	0.002%
69	10.631	2901	2905	2909	rBV	358	382	0.04%	0.003%
70	10.750	2929	2942	2953	rBV	248469	400377	42.12%	3.257%
71	10.817	2953	2963	2979	rVB	239170	387828	40.80%	3.155%
72	10.901	2986	2989	2992	rVV3	519	312	0.03%	0.003%
73	11.152	3063	3067	3071	rBV	314	291	0.03%	0.002%
74	11.174	3072	3074	3080	rVB2	303	221	0.02%	0.002%
75	11.463	3161	3164	3171	rBV3	365	390	0.04%	0.003%
76	11.669	3224	3228	3233	rBV2	310	234	0.02%	0.002%

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Instrument :
MSVOA_U
ClientSampleId :
XB504DL

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

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

77	11.740	3239	3250	3261	rBV	174977	281585	29.62%	2.291%
78	11.807	3261	3271	3303	rVB2	420794	950535	100.00%	7.733%
79	12.013	3332	3335	3340	rVB2	626	463	0.05%	0.004%
80	12.052	3344	3347	3350	rVV	245	217	0.02%	0.002%
81	12.142	3371	3375	3377	rBV3	346	330	0.03%	0.003%
82	12.193	3377	3391	3417	rBV2	397794	943392	99.25%	7.675%
83	12.467	3472	3476	3483	rBV4	956	1131	0.12%	0.009%
84	12.659	3533	3536	3540	rBV2	354	318	0.03%	0.003%
85	12.762	3565	3568	3569	rBV	446	225	0.02%	0.002%
86	12.801	3575	3580	3586	rVB3	411	576	0.06%	0.005%
87	12.836	3586	3591	3593	rBV	299	258	0.03%	0.002%
88	12.888	3602	3607	3609	rBV	226	227	0.02%	0.002%
89	12.991	3628	3639	3654	rBV2	58510	99412	10.46%	0.809%
90	13.454	3780	3783	3787	rBV2	233	219	0.02%	0.002%
91	13.833	3899	3901	3903	rBV2	412	217	0.02%	0.002%
92	13.907	3919	3924	3926	rBV2	468	399	0.04%	0.003%
93	14.016	3946	3958	3968	rBV2	185671	286785	30.17%	2.333%
94	14.084	3968	3979	4013	rVB	170636	305127	32.10%	2.482%
95	14.367	4064	4067	4069	rBV2	325	209	0.02%	0.002%
96	14.602	4135	4140	4145	rBV3	473	632	0.07%	0.005%
97	14.627	4145	4148	4150	rBV2	308	213	0.02%	0.002%
98	15.402	4384	4389	4390	rBV2	701	583	0.06%	0.005%
99	15.724	4486	4489	4492	rBV2	542	471	0.05%	0.004%
100	16.000	4572	4575	4577	rBV2	706	567	0.06%	0.005%

Sum of corrected areas: 12292156

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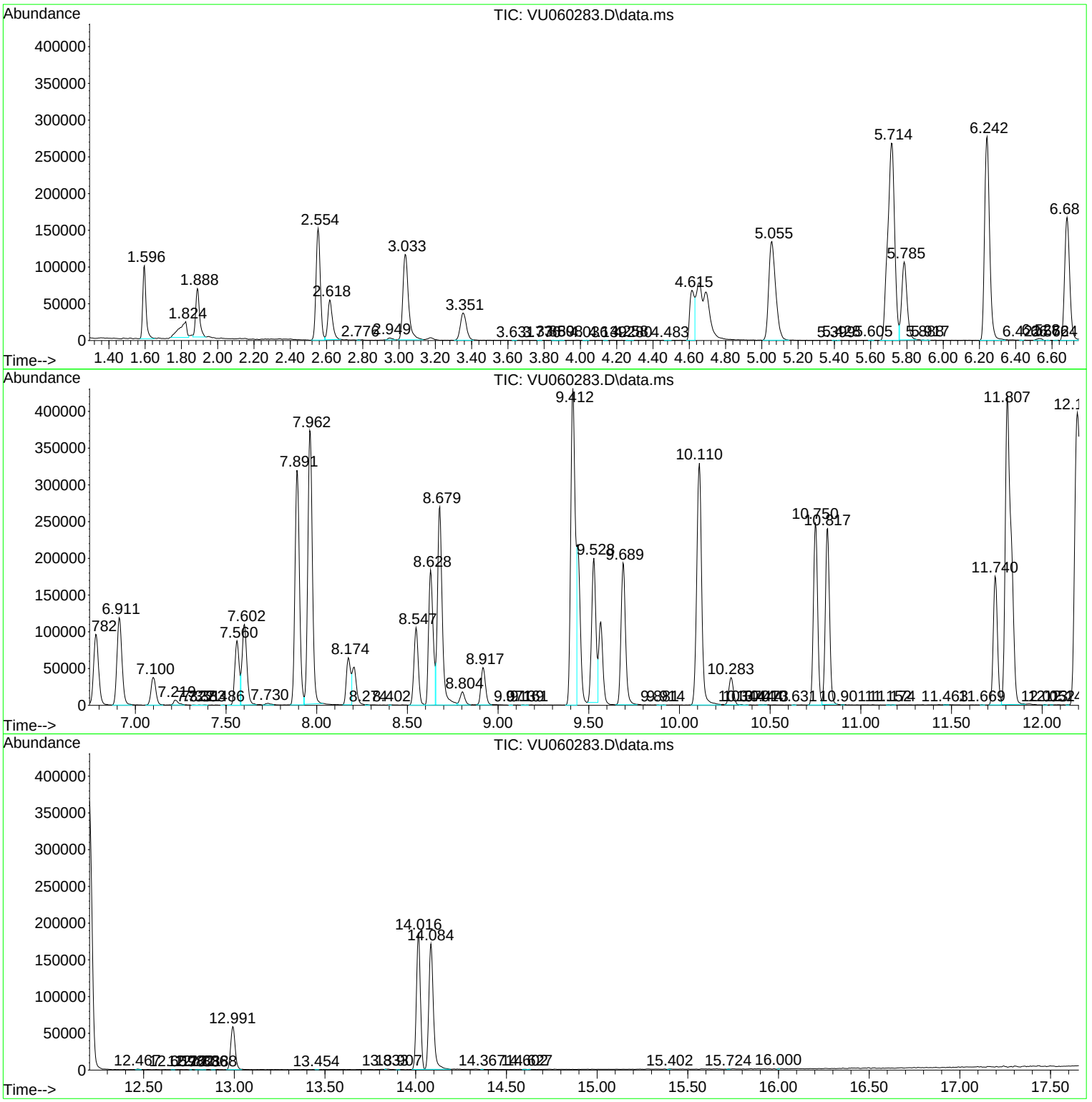
Instrument :
MSVOA_U
ClientSampleId :
XB504DL

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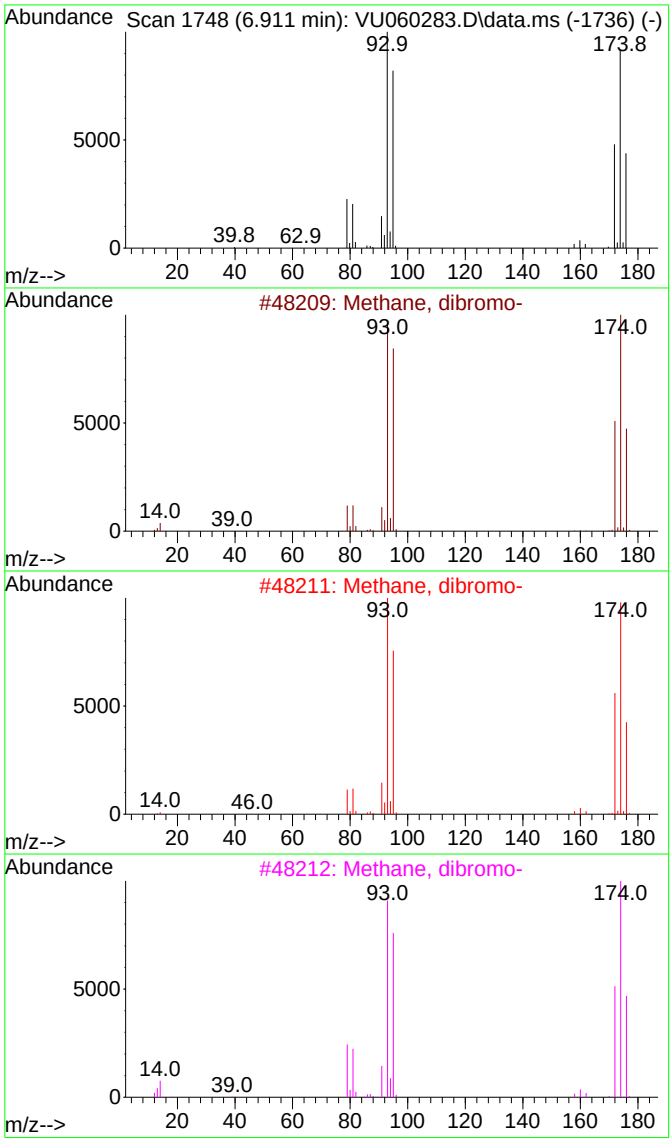
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.M
Quant Title : VOC Analysis

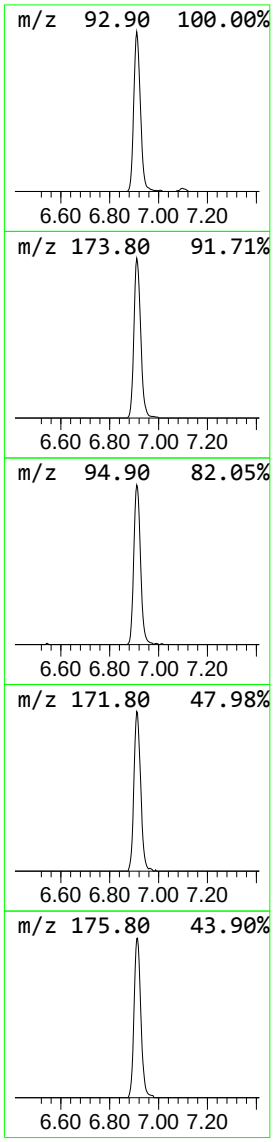
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Methane, dibromo- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.911	21.14 ug/L	227112	1,4-Difluorobenzene	6.242

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	3-Chloro-6-methoxy-4-methylpyrid...	174	C6H7ClN2O2	050450-89-0	9





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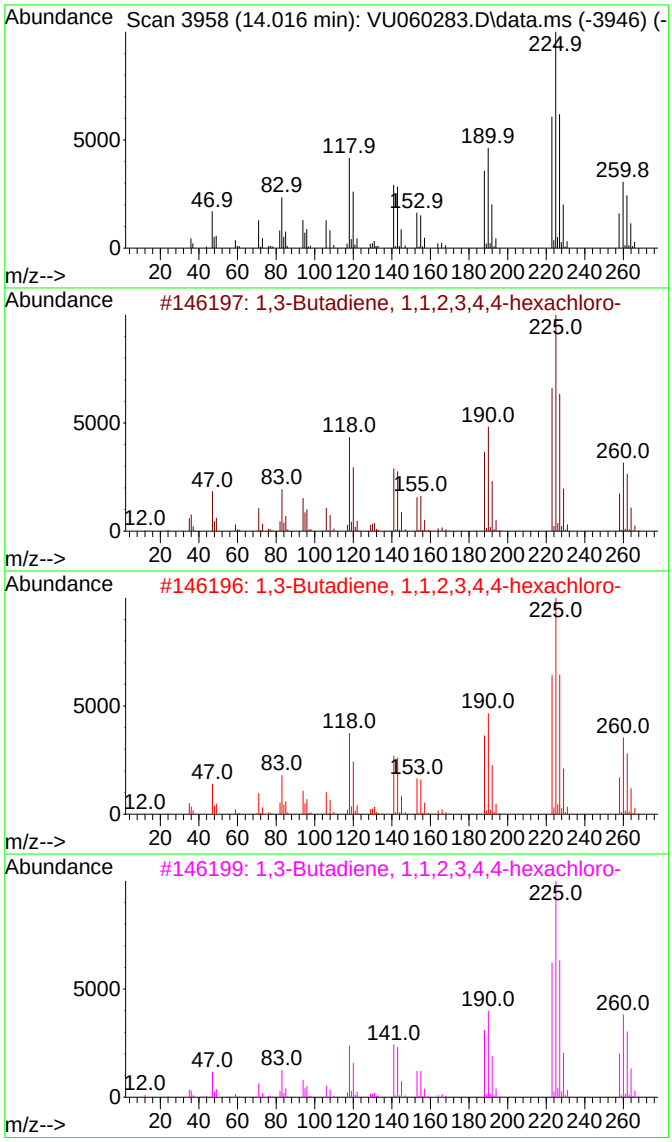
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.M
Quant Title : VOC Analysis

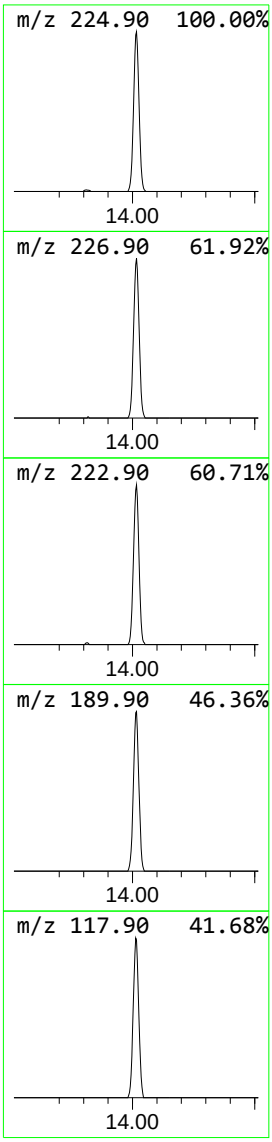
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.016	15.09 ug/L	286785	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	2-Chloro-9-methyl acridine	227	C14H10ClN	022684-24-8	11





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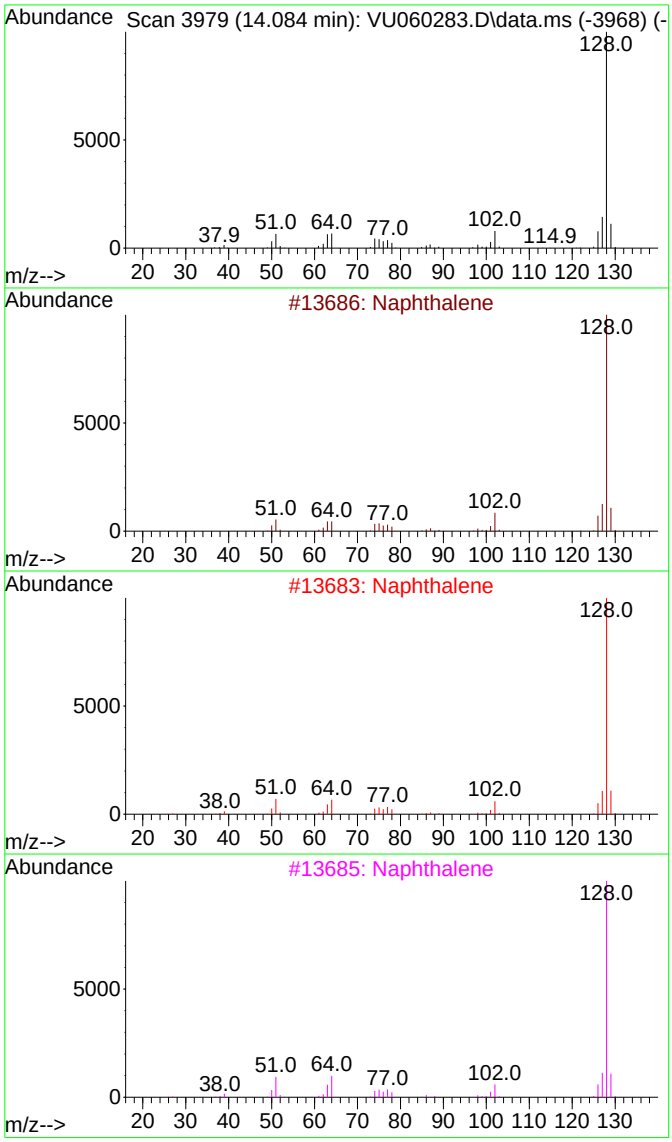
Quant Title : VOC Analysis

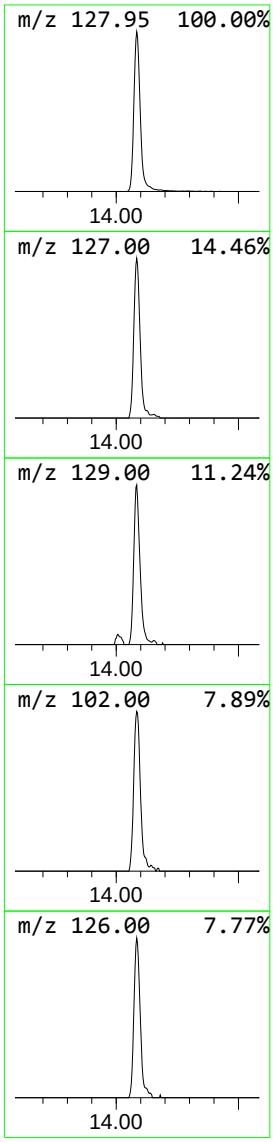
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Azulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.084	16.05 ug/L	305127	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	93
4	Azulene	128	C10H8	000275-51-4	91
5	1H-Indene, 1-methylene-	128	C10H8	002471-84-3	91





Tentatively Identified Compound (LSC) summary

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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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Methane, dibromo-	6.911	21.1	ug/L	227112	1	6.242	537177	50.0
1,3-Butadiene, ...	14.016	15.1	ug/L	286785	3	11.807	950535	50.0
Azulene	14.084	16.1	ug/L	305127	3	11.807	950535	50.0