LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072823\
Data File : VV031780.D
Acq On : 28 Jul 2023 11:59
Operator : SY/MD
Sample : 03805-01
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
X3H45

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_V\Method\SFAMVLM072523WMA.M
Title : VOC Analysis

Signal : TIC: VV031780.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.185	40	45	51	rBV	26972	24431	0.48%	0.039%
2	1.217	51	55	63	rVV3	7099	8472	0.17%	0.014%
3	1.278	67	74	93	rVV	190845	211085	4.16%	0.340%
4	1.484	131	138	146	rBV	213202	263258	5.19%	0.424%
5	1.529	146	152	172	rVB	188788	240683	4.75%	0.388%
6	1.712	199	209	227	rBV	924137	1231125	24.28%	1.983%
7	2.066	307	319	327	rBV3	795516	1313664	25.91%	2.116%
8	2.111	327	333	359	rVB	372983	584281	11.52%	0.941%
9	2.446	426	437	460	rBV	363611	593218	11.70%	0.955%
10	2.706	503	518	542	rBV	434911	903953	17.83%	1.456%
11	3.031	615	619	621	rBV5	1224	873	0.02%	0.001%
12	3.111	629	644	666	rBV	631332	1330925	26.25%	2.144%
13	3.413	733	738	742	rVB3	1036	840	0.02%	0.001%
14	3.619	798	802	806	rVB5	644	562	0.01%	0.001%
15	3.738	835	839	842	rVB3	976	569	0.01%	0.001%
16	3.789	842	855	884	rBV2	147974	437513	8.63%	0.705%
17	4.272	983	1005	1031	rBV3	678275	2266225	44.70%	3.650%
18	4.593	1103	1105	1110	rVB6	1753	1015	0.02%	0.002%
19	4.670	1126	1129	1131	rBV4	1370	981	0.02%	0.002%
20	4.738	1131	1150	1171	rVV2	259979	645802	12.74%	1.040%
21	4.960	1202	1219	1229	rBV2	593488	1579179	31.15%	2.543%
22	5.384	1348	1351	1353	rBV3	1382	747	0.01%	0.001%
23	5.478	1377	1380	1382	rBV4	1264	588	0.01%	0.001%
24	5.539	1386	1399	1421	rBV	424512	883937	17.44%	1.424%
25	5.838	1475	1492	1508	rBV4	146611	345267	6.81%	0.556%
26	5.992	1526	1540	1569	rBV	394318	842617	16.62%	1.357%
27	6.233	1603	1615	1633	rBV2	191922	382192	7.54%	0.616%
28	6.439	1667	1679	1696	rVV	88915	181796	3.59%	0.293%
29	6.574	1708	1721	1741	rBV3	15619	44265	0.87%	0.071%
30	6.703	1757	1761	1765	rBV6	1420	1415	0.03%	0.002%
31	6.793	1784	1789	1791	rVV3	1382	1251	0.02%	0.002%
32	6.822	1795	1798	1800	rBV3	991	682	0.01%	0.001%
33	6.857	1803	1809	1810	rBV4	1583	1373	0.03%	0.002%
34	6.918	1816	1828	1833	rBV	187416	313859	6.19%	0.506%
35	6.957	1834	1840	1869	rVV	373343	692162	13.65%	1.115%
36	7.085	1872	1880	1893	rBV	46229	90313	1.78%	0.145%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072823\
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Acq On : 28 Jul 2023 11:59
Operator : SY/MD
Sample : 03805-01
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : X3H45

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_V\Method\SFAMVLM072523WMA.M
Title : VOC Analysis

37	7.162	1893	1904	1919	rVV	809984	1425960	28.13%	2.297%
38	7.246	1920	1930	1955	rVB	692966	1259055	24.83%	2.028%
39	7.506	2008	2011	2013	rBV3	1157	617	0.01%	0.001%
40	7.584	2016	2035	2076	rBV2	1163230	2241605	44.21%	3.610%
41	7.773	2083	2094	2120	rVB	383001	671857	13.25%	1.082%
42	7.908	2124	2136	2163	rVB	907938	1558261	30.74%	2.510%
43	8.030	2164	2174	2182	rBV	534206	893001	17.61%	1.438%
44	8.079	2182	2189	2209	rVV	747961	1279278	25.23%	2.060%
45	8.178	2210	2220	2241	rVV	946141	1646811	32.48%	2.652%
46	8.284	2243	2253	2272	rVB	405968	691005	13.63%	1.113%
47	8.593	2339	2349	2357	rVB8	4638	8070	0.16%	0.013%
48	8.690	2376	2379	2382	rBV4	920	845	0.02%	0.001%
49	8.751	2390	2398	2399	rBV4	2101	2026	0.04%	0.003%
50	8.789	2399	2410	2417	rBV	734647	1286854	25.38%	2.073%
51	8.911	2436	2448	2454	rBV	1377784	2244670	44.27%	3.615%
52	8.950	2454	2460	2484	rVB	2055576	3098354	61.11%	4.990%
53	9.075	2488	2499	2520	rBV	2065518	3292314	64.94%	5.303%
54	9.339	2579	2581	2588	rVB6	1522	1331	0.03%	0.002%
55	9.490	2613	2628	2667	rBV4	2341892	5069855	100.00%	8.166%
56	9.796	2721	2723	2730	rVB8	1498	1419	0.03%	0.002%
57	10.027	2792	2795	2797	rBV3	990	666	0.01%	0.001%
58	10.043	2797	2800	2803	rVV3	1625	994	0.02%	0.002%
59	10.091	2813	2815	2819	rBV4	1182	788	0.02%	0.001%
60	10.156	2824	2835	2844	rVV	602440	936702	18.48%	1.509%
61	10.214	2844	2853	2873	rVB	573889	911872	17.99%	1.469%
62	10.481	2925	2936	2953	rBV	280087	429880	8.48%	0.692%
63	10.680	2991	2998	2999	rBV7	4609	4449	0.09%	0.007%
64	10.805	3033	3037	3040	rBV5	2432	2412	0.05%	0.004%
65	10.857	3042	3053	3078	rVV	994452	1501314	29.61%	2.418%
66	11.063	3114	3117	3119	rBV3	1379	673	0.01%	0.001%
67	11.136	3132	3140	3145	rBV6	3643	4176	0.08%	0.007%
68	11.210	3145	3163	3187	rBV2	2343438	4772329	94.13%	7.687%
69	11.464	3239	3242	3243	rBV2	1604	738	0.01%	0.001%
70	11.500	3250	3253	3255	rBV3	1329	1050	0.02%	0.002%
71	11.580	3262	3278	3304	rBV2	1815443	3846995	75.88%	6.196%
72	11.844	3349	3360	3370	rVV6	21111	36984	0.73%	0.060%
73	11.882	3370	3372	3375	rVB4	1404	645	0.01%	0.001%
74	11.972	3398	3400	3406	rVB4	1270	995	0.02%	0.002%
75	12.014	3410	3413	3414	rBV	1155	672	0.01%	0.001%
76	12.371	3512	3524	3539	rBV	311819	500846	9.88%	0.807%

LSC Area Percent Report

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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
X3H45

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_V\Method\SFAMVLM072523WMA.M
Title : VOC Analysis

77	12.519	3567	3570	3572	rBV4	1085	714	0.01%	0.001%
78	12.554	3577	3581	3584	rBV6	1086	826	0.02%	0.001%
79	12.593	3588	3593	3596	rBV7	2545	2139	0.04%	0.003%
80	12.657	3610	3613	3618	rBV5	1644	1496	0.03%	0.002%
81	12.747	3638	3641	3642	rBV3	1741	908	0.02%	0.001%
82	13.046	3732	3734	3736	rBV2	930	587	0.01%	0.001%
83	13.082	3738	3745	3747	rBV7	2707	2930	0.06%	0.005%
84	13.204	3768	3783	3805	rBV	632026	993276	19.59%	1.600%
85	13.320	3817	3819	3821	rVB3	1273	549	0.01%	0.001%
86	13.387	3824	3840	3850	rBV	2878985	4376500	86.32%	7.049%
87	13.445	3850	3858	3878	rVB	1076395	1634557	32.24%	2.633%
88	13.686	3927	3933	3942	rVB	6558	8979	0.18%	0.014%
89	13.792	3964	3966	3969	rBV3	1011	608	0.01%	0.001%
90	13.879	3988	3993	4000	rBV7	2858	4233	0.08%	0.007%
91	13.931	4006	4009	4013	rBV4	1242	958	0.02%	0.002%
92	14.175	4082	4085	4089	rVB4	1016	615	0.01%	0.001%
93	14.236	4102	4104	4109	rBV4	1051	812	0.02%	0.001%
94	14.381	4145	4149	4150	rBV4	1513	972	0.02%	0.002%
95	14.522	4191	4193	4194	rBV2	1375	564	0.01%	0.001%
96	14.699	4244	4248	4251	rBV5	1902	1563	0.03%	0.003%
97	14.853	4293	4296	4297	rBV2	1414	880	0.02%	0.001%
98	14.934	4319	4321	4323	rBV3	1490	667	0.01%	0.001%
99	15.066	4359	4362	4363	rBV3	1369	816	0.02%	0.001%
100	15.516	4499	4502	4505	rBV5	1889	1507	0.03%	0.002%

Sum of corrected areas: 62087142

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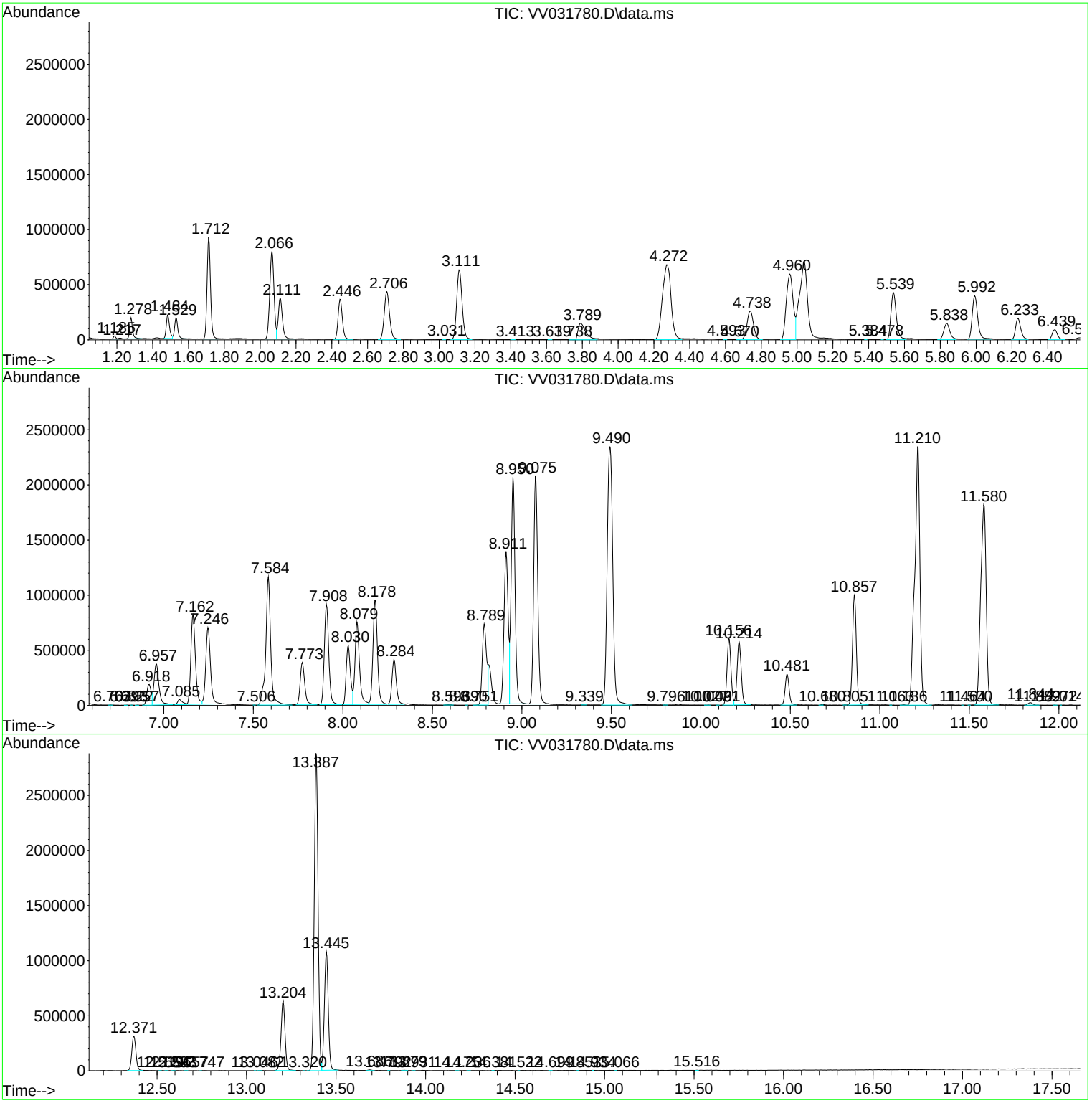
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
X3H45

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.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_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

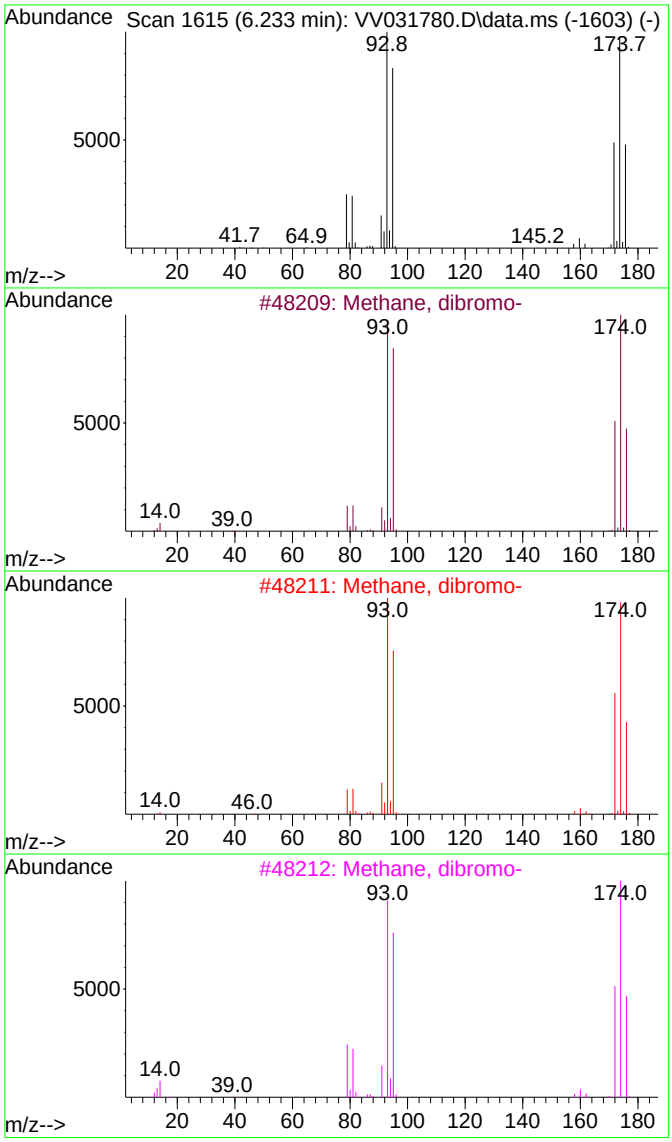
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

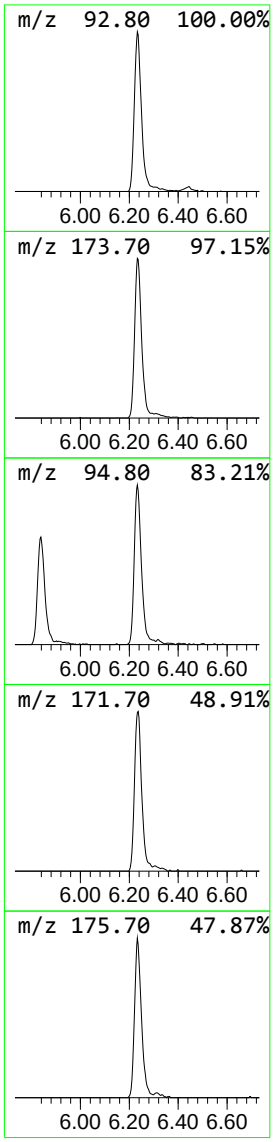
****

Peak Number 1 Methane, dibromo- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.233	21.62 ug/L	382192	1,4-Difluorobenzene	5.539

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	95
3	Methane, dibromo-	172	CH2Br2	000074-95-3	94
4	Methane, dibromo-	172	CH2Br2	000074-95-3	91
5	6-Bromo-2-pyridinamine	172	C5H5BrN2	019798-81-3	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072823\
Data File : VV031780.D
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
X3H45

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

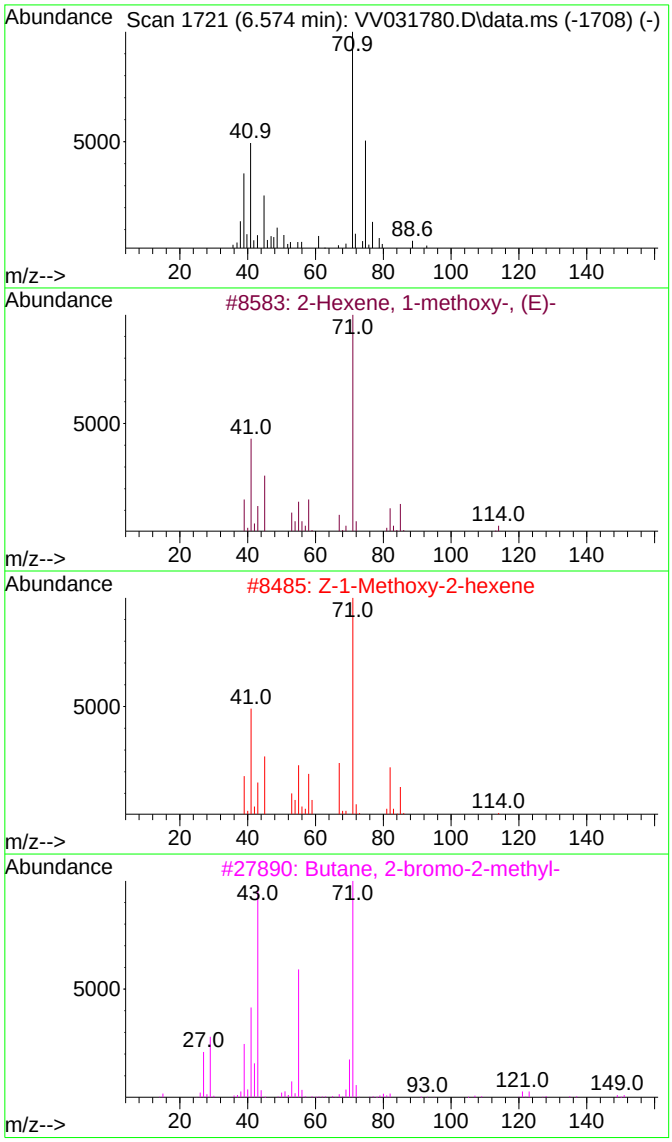
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

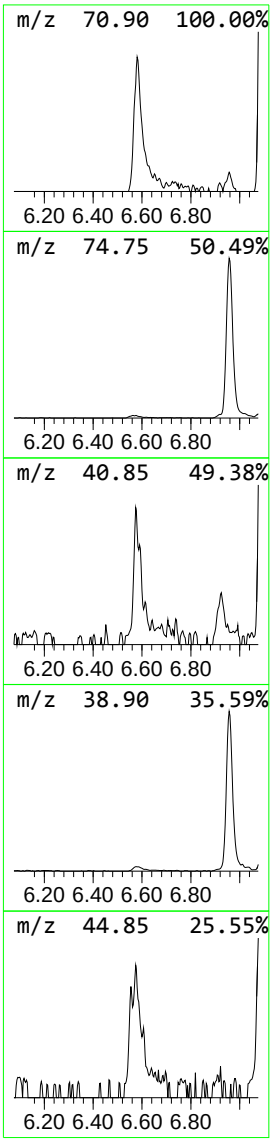
****

Peak Number 2 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.574	2.50 ug/L	44265	1,4-Difluorobenzene	5.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexene, 1-methoxy-, (E)-	114	C7H14O	056052-83-6	25
2	Z-1-Methoxy-2-hexene	114	C7H14O	1000279-60-9	25
3	Butane, 2-bromo-2-methyl-	150	C5H11Br	000507-36-8	17
4	Chloromethyl cyanide	75	C2H2ClN	000107-14-2	14
5	Mercaptamine	77	C2H7NS	000060-23-1	9





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Data File : VV031780.D
Acq On : 28 Jul 2023 11:59
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
X3H45

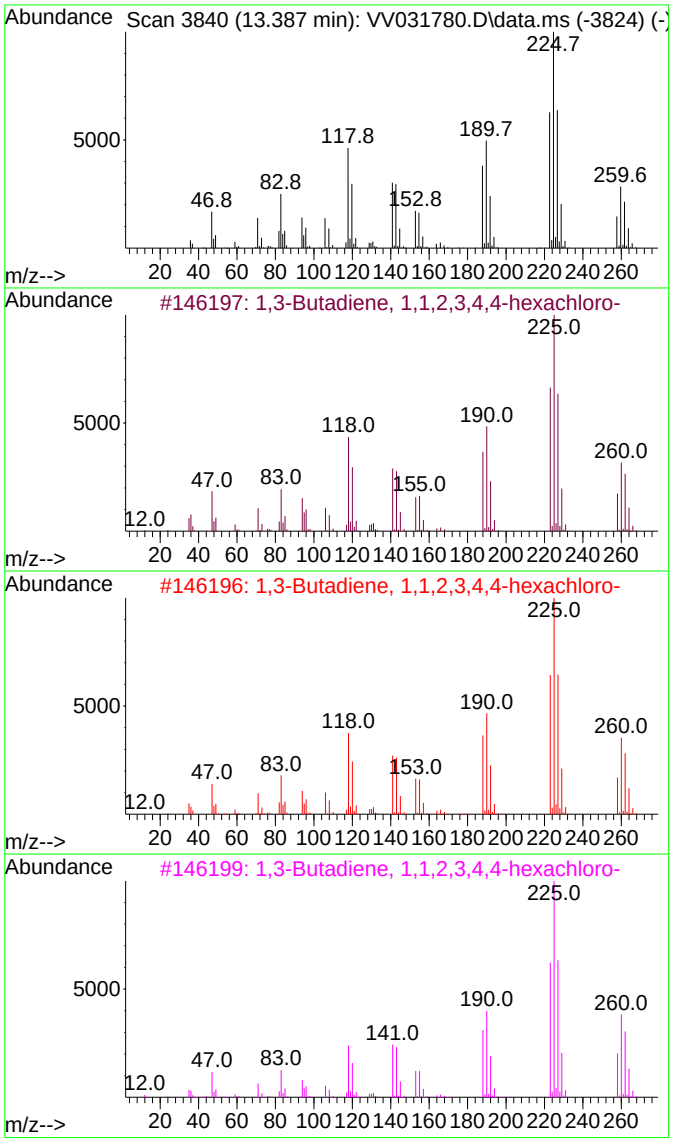
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

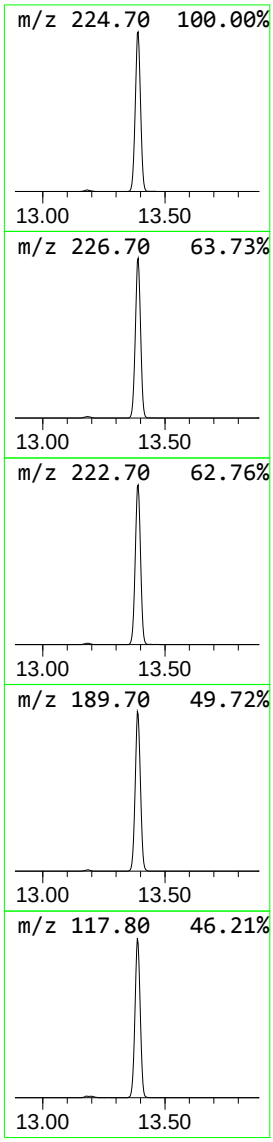
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.387	45.85 ug/L	4376500	1,4-Dichlorobenzene-d4	11.191

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	25





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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
X3H45

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

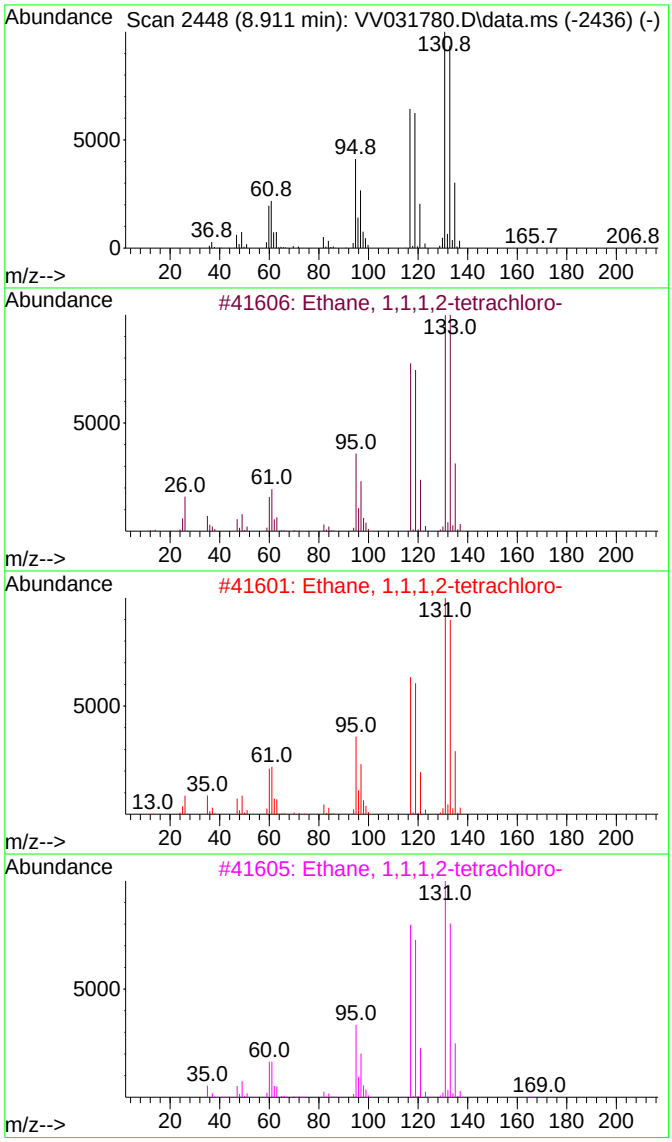
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

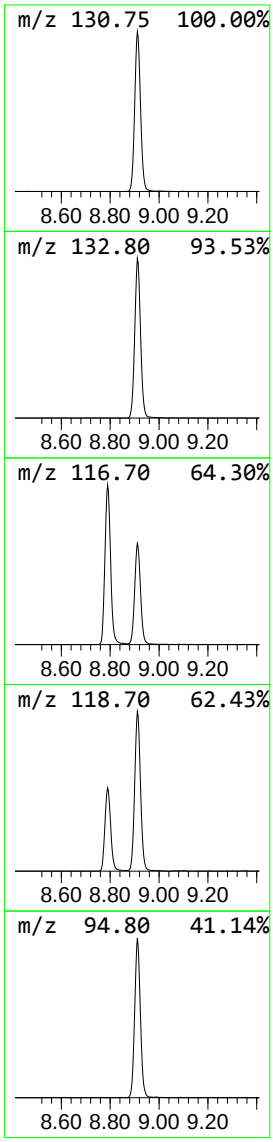
****

Peak Number 6 Ethane, 1,1,1,2-tetrachloro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.911	87.22 ug/L	2244670	Chlorobenzene-d5	8.789

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	91
2	Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	91
3	Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	86
4	Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	64
5	Trichloroacetyl chloride	180	C2Cl4O	000076-02-8	11





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072823\
Data File : VV031780.D
Acq On : 28 Jul 2023 11:59
Operator : SY/MD
Sample : 03805-01
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
X3H45

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.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-	6.233	21.6	ug/L	382192	1	5.539	883937	50.0
unknown-01	6.574	2.5	ug/L	44265	1	5.539	883937	50.0
1,3-Butadiene, ...	13.387	45.9	ug/L	4376500	3	11.191	4772330	50.0
Ethane, 1,1,1,2...	8.911	87.2	ug/L	2244670	2	8.789	1286850	50.0