LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV070323\
Data File : VV031636.D
Acq On : 03 Jul 2023 14:46
Operator : SY/MD
Sample : 03444-22ME
Misc : 4.74g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
A46Y3ME

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\SFAMVLM061423WMA.M
Title : VOC Analysis

Signal : TIC: VV031636.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.278	68	74	96	rVB2	106299	185803	10.27%	1.559%
2	2.037	300	310	329	rVB	204447	321337	17.75%	2.696%
3	2.394	410	421	430	rBV2	9592	21544	1.19%	0.181%
4	2.500	450	454	459	rVB5	914	971	0.05%	0.008%
5	2.561	459	473	486	rBV2	9918	22892	1.26%	0.192%
6	2.687	502	512	528	rVB2	5563	10633	0.59%	0.089%
7	2.802	544	548	552	rVB2	544	542	0.03%	0.005%
8	2.954	587	595	610	rVB8	2715	5626	0.31%	0.047%
9	3.108	632	643	661	rVB2	17222	37129	2.05%	0.311%
10	3.648	807	811	815	rVB4	701	580	0.03%	0.005%
11	3.812	848	862	896	rBV2	196238	557990	30.83%	4.681%
12	4.253	981	999	1025	rBV2	126043	346696	19.15%	2.908%
13	4.513	1063	1080	1103	rBV2	69808	189386	10.46%	1.589%
14	4.632	1114	1117	1123	rVB4	699	758	0.04%	0.006%
15	4.815	1163	1174	1175	rBV7	1163	1468	0.08%	0.012%
16	4.851	1182	1185	1188	rBV2	561	431	0.02%	0.004%
17	4.957	1202	1218	1265	rBV2	304477	797040	44.03%	6.686%
18	5.224	1298	1301	1303	rBV	609	400	0.02%	0.003%
19	5.410	1352	1359	1369	rVV7	2220	3993	0.22%	0.033%
20	5.478	1376	1380	1382	rBV2	516	403	0.02%	0.003%
21	5.539	1385	1399	1425	rBV	289407	634585	35.06%	5.323%
22	5.670	1438	1440	1442	rBV3	772	387	0.02%	0.003%
23	5.754	1463	1466	1469	rBV3	520	385	0.02%	0.003%
24	5.780	1470	1474	1475	rVV4	1168	886	0.05%	0.007%
25	5.793	1475	1478	1481	rVV3	1948	1784	0.10%	0.015%
26	5.841	1481	1493	1515	rVB6	22721	52716	2.91%	0.442%
27	5.995	1526	1541	1570	rBV	172386	399101	22.05%	3.348%
28	6.381	1658	1661	1663	rBV3	660	391	0.02%	0.003%
29	6.580	1719	1723	1727	rBV4	556	623	0.03%	0.005%
30	6.674	1749	1752	1756	rBV3	720	464	0.03%	0.004%
31	6.693	1756	1758	1764	rVB5	830	603	0.03%	0.005%
32	6.786	1784	1787	1794	rVB3	743	594	0.03%	0.005%
33	6.844	1802	1805	1808	rBV3	916	710	0.04%	0.006%
34	6.921	1818	1829	1854	rVV	83654	172818	9.55%	1.450%
35	7.114	1886	1889	1892	rVB2	545	412	0.02%	0.003%
36	7.195	1905	1914	1920	rBV9	3396	6230	0.34%	0.052%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV070323\
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Operator : SY/MD
Sample : 03444-22ME
Misc : 4.74g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
A46Y3ME

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\SFAMVLM061423WMA.M
Title : VOC Analysis

37	7.249	1920	1931	1944	rVV	297735	530051	29.28%	4.446%
38	7.323	1945	1954	1975	rVB	129027	243336	13.44%	2.041%
39	7.506	2006	2011	2017	rVB9	1722	2065	0.11%	0.017%
40	7.561	2018	2028	2051	rBV	61359	129049	7.13%	1.083%
41	7.722	2072	2078	2085	rVB8	1925	3101	0.17%	0.026%
42	7.793	2095	2100	2104	rBV6	939	867	0.05%	0.007%
43	7.912	2124	2137	2151	rBV2	82579	145338	8.03%	1.219%
44	7.998	2162	2164	2167	rBV3	535	453	0.03%	0.004%
45	8.050	2167	2180	2208	rBV3	137417	406559	22.46%	3.411%
46	8.281	2249	2252	2263	rVB7	1845	2192	0.12%	0.018%
47	8.375	2276	2281	2282	rBV2	669	592	0.03%	0.005%
48	8.535	2327	2331	2335	rVB6	935	884	0.05%	0.007%
49	8.648	2364	2366	2372	rVB2	517	470	0.03%	0.004%
50	8.793	2398	2411	2436	rBV	441056	803873	44.41%	6.743%
51	8.953	2451	2461	2481	rBV	97177	170850	9.44%	1.433%
52	9.079	2490	2500	2520	rBV	114888	205624	11.36%	1.725%
53	9.256	2553	2555	2561	rVB	1001	723	0.04%	0.006%
54	9.288	2561	2565	2570	rBV3	709	657	0.04%	0.006%
55	9.368	2586	2590	2593	rBV2	600	613	0.03%	0.005%
56	9.413	2598	2604	2606	rBV5	1600	1596	0.09%	0.013%
57	9.490	2617	2628	2643	rBV3	22321	40395	2.23%	0.339%
58	9.622	2663	2669	2670	rVV5	1231	1132	0.06%	0.009%
59	9.648	2671	2677	2686	rVB8	3314	5365	0.30%	0.045%
60	9.725	2698	2701	2702	rBV2	1220	645	0.04%	0.005%
61	9.796	2717	2723	2729	rVB5	1084	1678	0.09%	0.014%
62	9.873	2743	2747	2749	rBV3	1790	1432	0.08%	0.012%
63	9.963	2765	2775	2789	rBV2	11326	19621	1.08%	0.165%
64	10.063	2802	2806	2808	rBV4	1279	1048	0.06%	0.009%
65	10.165	2821	2838	2860	rBV	277107	466910	25.80%	3.917%
66	10.301	2872	2880	2894	rVB2	11947	19043	1.05%	0.160%
67	10.397	2900	2910	2914	rBV3	20493	32379	1.79%	0.272%
68	10.487	2930	2938	2947	rBV2	7541	11223	0.62%	0.094%
69	10.635	2981	2984	2985	rBV	912	608	0.03%	0.005%
70	10.686	2985	3000	3015	rVB5	6849	14965	0.83%	0.126%
71	10.821	3037	3042	3044	rVV5	1315	1262	0.07%	0.011%
72	10.863	3047	3055	3074	rVB2	31678	51819	2.86%	0.435%
73	11.001	3082	3098	3103	rBV2	12446	22861	1.26%	0.192%
74	11.085	3120	3124	3126	rBV4	872	644	0.04%	0.005%
75	11.143	3133	3142	3147	rBV9	4416	6377	0.35%	0.053%
76	11.194	3147	3158	3177	rVV	565490	881716	48.71%	7.396%

LSC Area Percent Report

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Operator : SY/MD
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Misc : 4.74g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : A46Y3ME

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\SFAMVLM061423WMA.M
Title : VOC Analysis

77	11.288	3180	3187	3195	rVB4	6902	11478	0.63%	0.096%
78	11.493	3238	3251	3265	rBV	1095267	1596424	88.20%	13.392%
79	11.574	3265	3276	3300	rVV2	1057424	1810056	100.00%	15.184%
80	11.693	3302	3313	3328	rVV	78306	123662	6.83%	1.037%
81	11.863	3358	3366	3368	rBV4	8751	11550	0.64%	0.097%
82	11.963	3390	3397	3416	rVB2	13395	27895	1.54%	0.234%
83	12.066	3421	3429	3434	rBV5	4699	6939	0.38%	0.058%
84	12.204	3464	3472	3478	rVB9	4502	6886	0.38%	0.058%
85	12.252	3483	3487	3497	rVB8	2960	4613	0.25%	0.039%
86	12.320	3499	3508	3515	rBV9	3272	6412	0.35%	0.054%
87	12.413	3530	3537	3545	rVB6	6715	8969	0.50%	0.075%
88	12.500	3557	3564	3571	rBV9	4407	6257	0.35%	0.052%
89	12.664	3611	3615	3616	rBV3	1891	1383	0.08%	0.012%
90	12.741	3633	3639	3643	rBV9	2952	3535	0.20%	0.030%
91	12.831	3661	3667	3675	rVB9	4928	7464	0.41%	0.063%
92	12.998	3709	3719	3723	rBV9	4729	8304	0.46%	0.070%
93	13.214	3777	3786	3793	rBV8	3633	6596	0.36%	0.055%
94	13.452	3852	3860	3871	rBV2	11363	18649	1.03%	0.156%
95	14.159	4077	4080	4085	rBV6	1283	900	0.05%	0.008%
96	14.583	4206	4212	4215	rBV7	3798	4710	0.26%	0.040%
97	14.715	4250	4253	4254	rBV2	1135	628	0.03%	0.005%
98	15.763	4573	4579	4585	rBV9	2092	2931	0.16%	0.025%
99	16.397	4768	4776	4791	rVB	48913	76061	4.20%	0.638%
100	17.480	5104	5113	5129	rVB3	95120	160108	8.85%	1.343%

Sum of corrected areas: 11920737

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV070323\
Data File : VV031636.D
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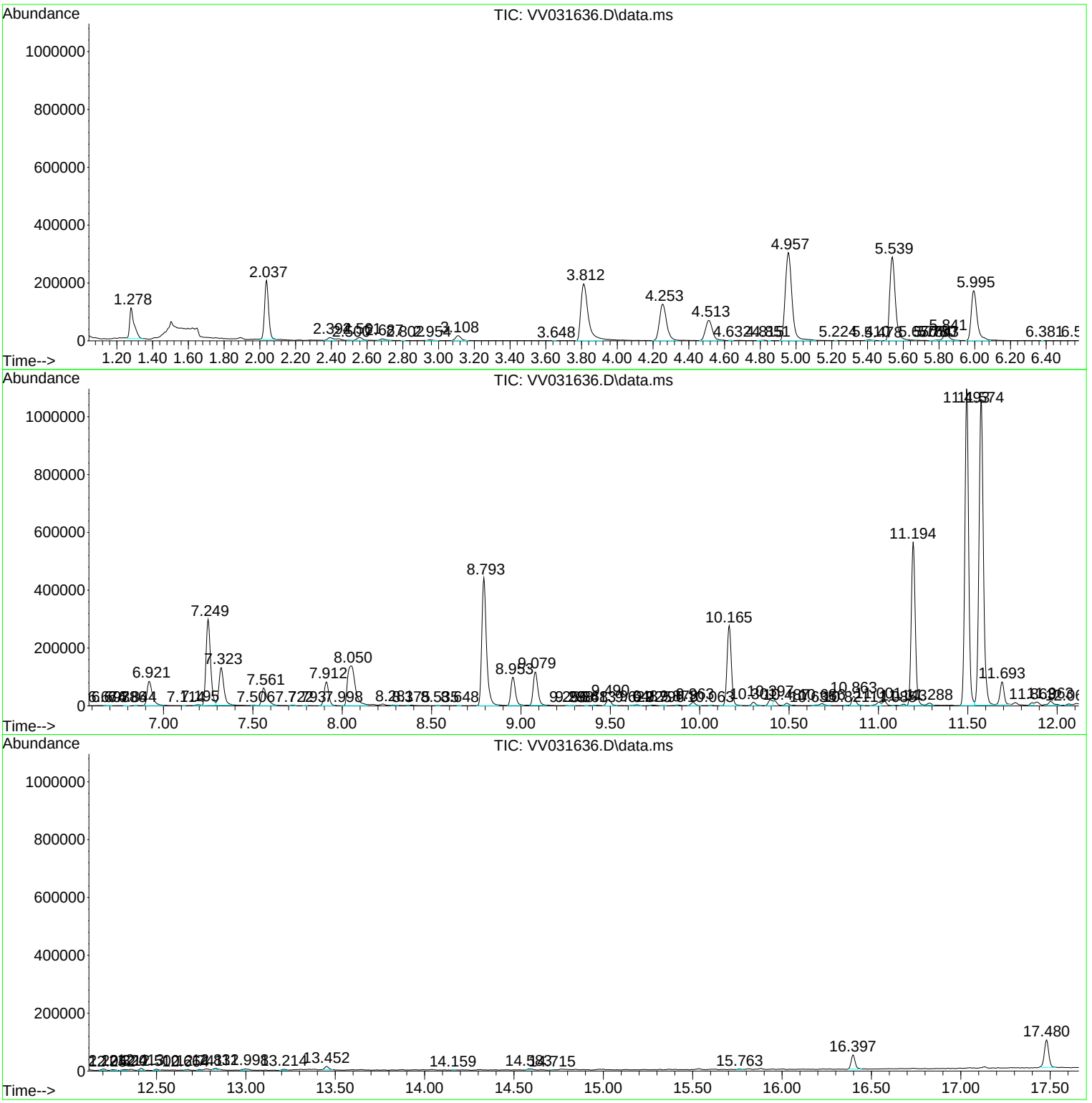
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
A46Y3ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV070323\
Data File : VV031636.D
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Operator : SY/MD
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Instrument :
MSVOA_V
ClientSampleId :
A46Y3ME

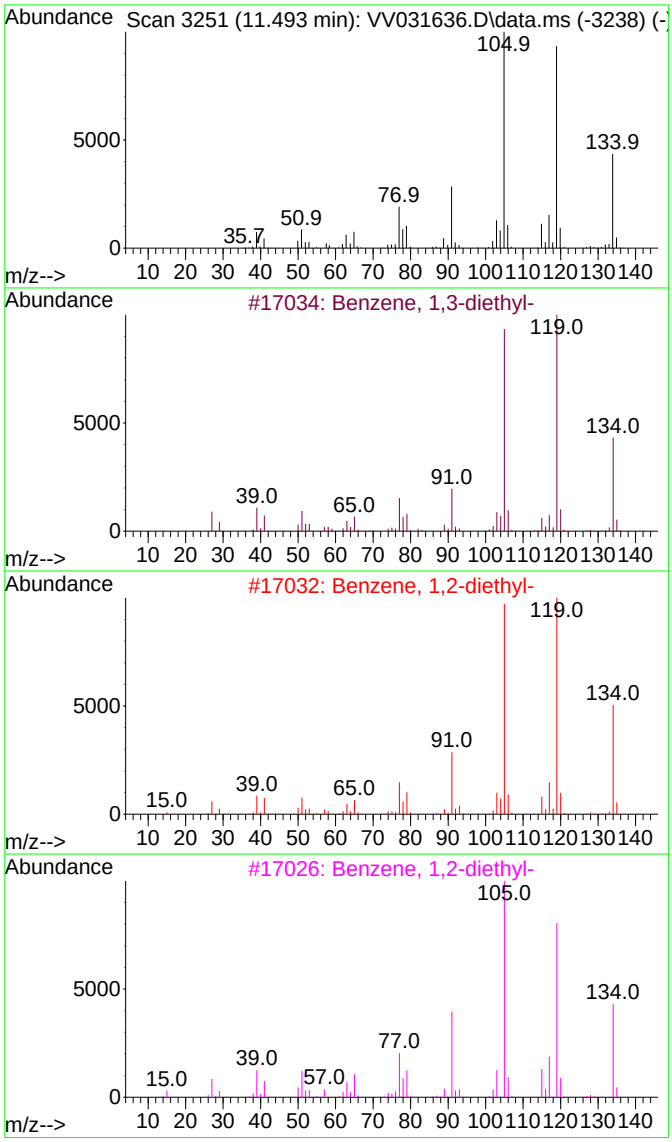
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.M
Quant Title : VOC Analysis

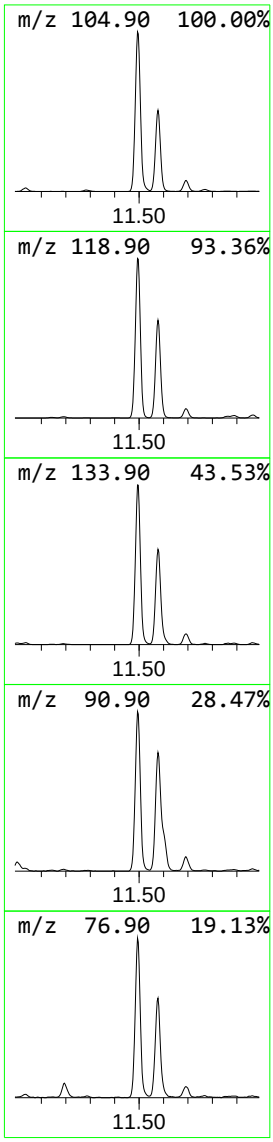
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzene, 1,3-diethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.493	90.53 ug/L	1596420	1,4-Dichlorobenzene-d4	11.194

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	97
2	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	96
3	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	96
4	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	96
5	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV070323\
Data File : VV031636.D
Acq On : 03 Jul 2023 14:46
Operator : SY/MD
Sample : 03444-22ME
Misc : 4.74g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
A46Y3ME

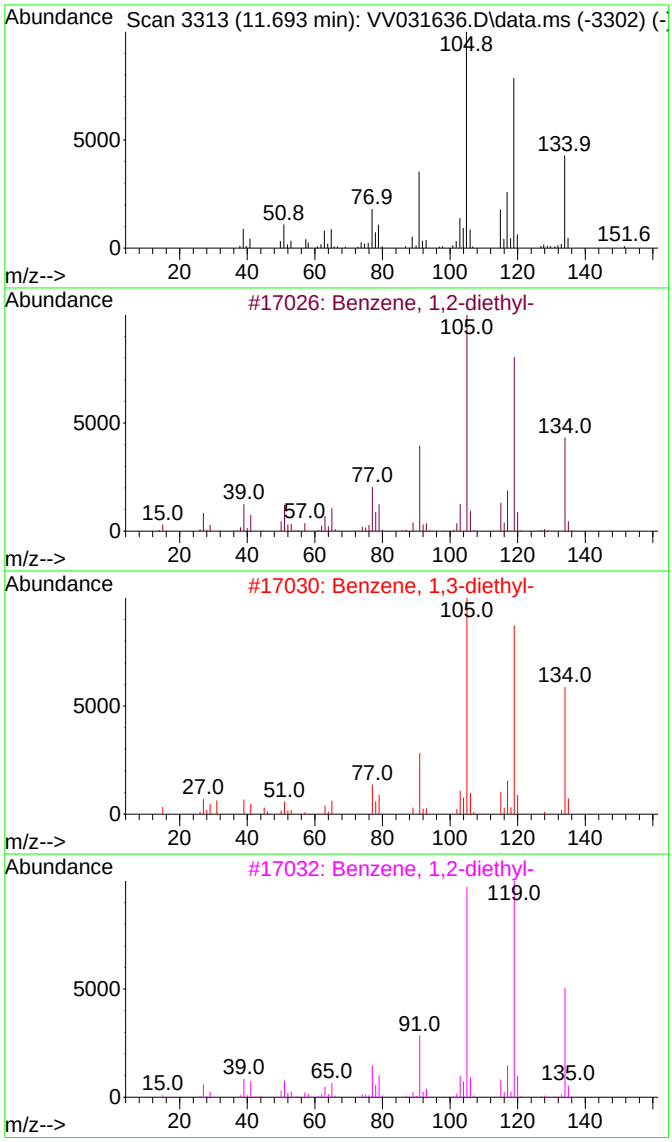
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.M
Quant Title : VOC Analysis

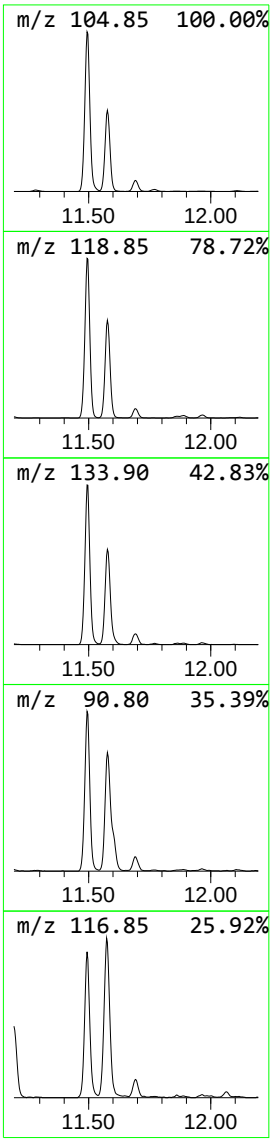
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, 1,2-diethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.693	7.01 ug/L	123662	1,4-Dichlorobenzene-d4	11.194

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	94
2	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	90
3	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	90
4	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	83
5	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV070323\
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Operator : SY/MD
Sample : 03444-22ME
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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
A46Y3ME

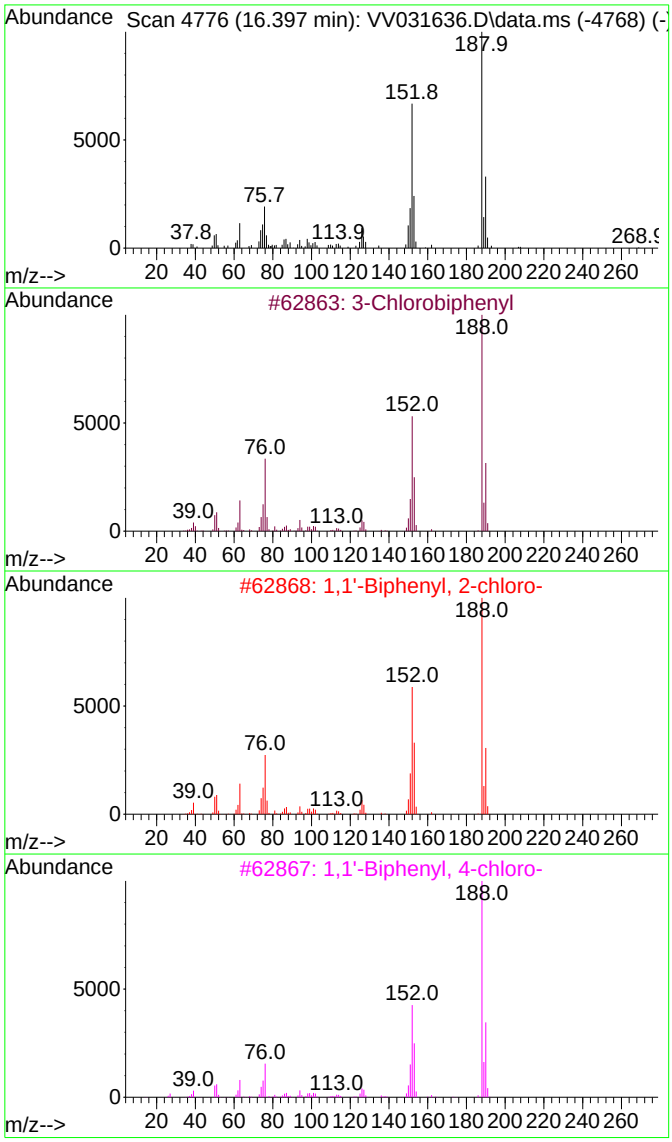
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.M
Quant Title : VOC Analysis

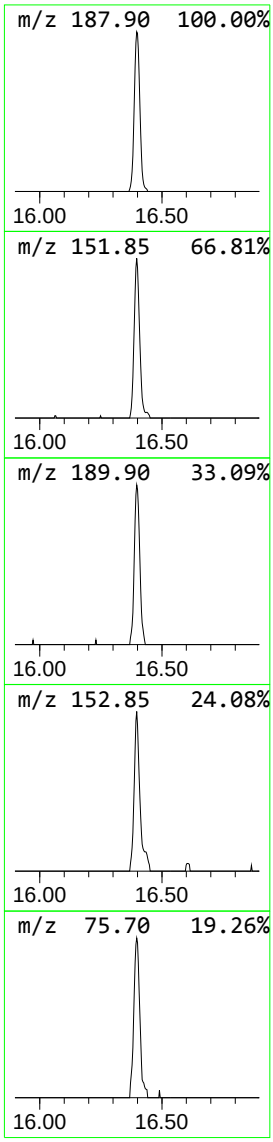
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 3-Chlorobiphenyl Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.397	4.31 ug/L	76061	1,4-Dichlorobenzene-d4	11.194

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chlorobiphenyl	188	C12H9Cl	002051-61-8	97
2	1,1'-Biphenyl, 2-chloro-	188	C12H9Cl	002051-60-7	97
3	1,1'-Biphenyl, 4-chloro-	188	C12H9Cl	002051-62-9	96
4	3-Chlorobiphenyl	188	C12H9Cl	002051-61-8	96
5	1,1'-Biphenyl, 4-chloro-	188	C12H9Cl	002051-62-9	95





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Operator : SY/MD
Sample : 03444-22ME
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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
A46Y3ME

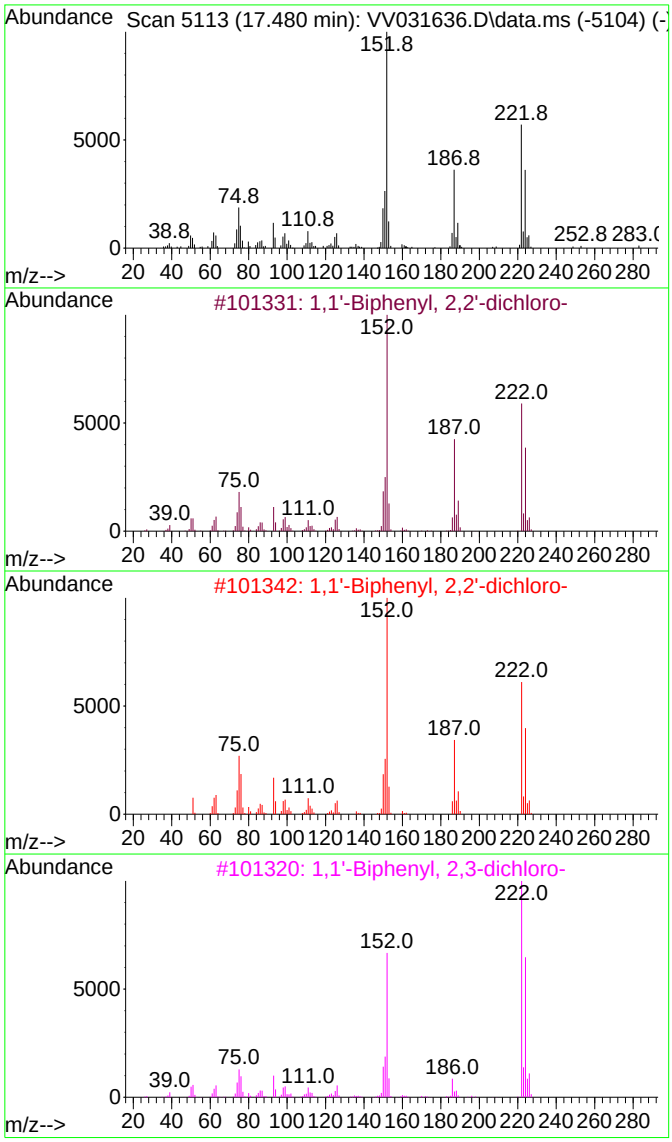
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.M
Quant Title : VOC Analysis

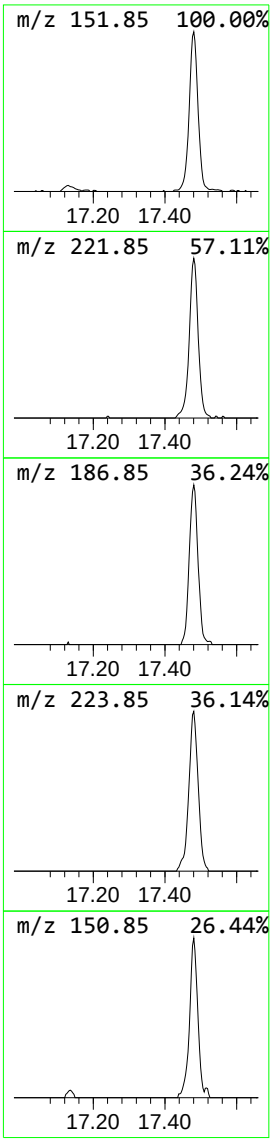
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1,1'-Biphenyl, 2,2'-dichloro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.480	9.08 ug/L	160108	1,4-Dichlorobenzene-d4	11.194

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 2,2'-dichloro-	222	C12H8Cl2	013029-08-8	99
2	1,1'-Biphenyl, 2,2'-dichloro-	222	C12H8Cl2	013029-08-8	98
3	1,1'-Biphenyl, 2,3-dichloro-	222	C12H8Cl2	016605-91-7	98
4	1,1'-Biphenyl, 2,4'-dichloro-	222	C12H8Cl2	034883-43-7	98
5	1,1'-Biphenyl, 3,4'-dichloro-	222	C12H8Cl2	002974-90-5	98





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV070323\
Data File : VV031636.D
Acq On : 03 Jul 2023 14:46
Operator : SY/MD
Sample : 03444-22ME
Misc : 4.74g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
A46Y3ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.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
Benzene, 1,3-di...	11.493	90.5	ug/L	1596420	3	11.194	881716	50.0
Benzene, 1,2-di...	11.693	7.0	ug/L	123662	3	11.194	881716	50.0
3-Chlorobiphenyl	16.397	4.3	ug/L	76061	3	11.194	881716	50.0
1,1'-Biphenyl, ...	17.480	9.1	ug/L	160108	3	11.194	881716	50.0