LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
Data File : VU059332.D
Acq On : 18 Jun 2024 23:25
Operator : MD/SY
Sample : P2873-03 200X
Misc : 2.64g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0SG7

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\SFAMULM052924WMA.M
Title : VOC Analysis

Signal : TIC: VU059332.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	88	95	108	rBV	49640	58418	4.02%	0.746%
2	1.908	184	192	209	rVB	47779	64586	4.45%	0.825%
3	2.560	384	395	408	rBV	80469	132622	9.13%	1.695%
4	2.721	443	445	448	rBV2	168	96	0.01%	0.001%
5	2.917	498	506	509	rBV3	524	715	0.05%	0.009%
6	3.039	528	544	563	rBV2	28766	55103	3.79%	0.704%
7	3.171	578	585	586	rBV2	508	494	0.03%	0.006%
8	3.216	596	599	601	rBV	255	198	0.01%	0.003%
9	3.383	648	651	653	rBV	203	153	0.01%	0.002%
10	3.428	660	665	668	rBV2	236	295	0.02%	0.004%
11	3.612	718	722	730	rBV2	189	276	0.02%	0.004%
12	3.663	735	738	742	rBV2	318	292	0.02%	0.004%
13	3.837	788	792	795	rBV	164	184	0.01%	0.002%
14	3.940	822	824	827	rBV2	187	119	0.01%	0.002%
15	3.988	834	839	841	rBV	149	147	0.01%	0.002%
16	4.039	851	855	857	rBV	178	174	0.01%	0.002%
17	4.290	930	933	935	rBV2	198	123	0.01%	0.002%
18	4.309	936	939	941	rBV2	230	154	0.01%	0.002%
19	4.419	968	973	975	rBV	368	287	0.02%	0.004%
20	4.525	1002	1006	1010	rBV2	236	247	0.02%	0.003%
21	4.615	1024	1034	1062	rBV	50341	123934	8.53%	1.584%
22	4.933	1129	1133	1136	rBV3	320	367	0.03%	0.005%
23	5.055	1156	1171	1200	rBV	83500	188187	12.96%	2.405%
24	5.239	1221	1228	1232	rBV2	238	390	0.03%	0.005%
25	5.296	1243	1246	1247	rVV	208	115	0.01%	0.001%
26	5.325	1251	1255	1257	rBV2	165	144	0.01%	0.002%
27	5.380	1267	1272	1273	rBV	200	173	0.01%	0.002%
28	5.396	1275	1277	1279	rBV	173	89	0.01%	0.001%
29	5.412	1279	1282	1283	rBV	148	89	0.01%	0.001%
30	5.550	1321	1325	1329	rBV2	210	223	0.02%	0.003%
31	5.718	1357	1377	1409	rBV3	165147	460038	31.67%	5.878%
32	5.911	1430	1437	1439	rBV3	425	464	0.03%	0.006%
33	5.981	1457	1459	1462	rVB2	211	120	0.01%	0.002%
34	6.001	1462	1465	1466	rBV	357	181	0.01%	0.002%
35	6.091	1488	1493	1497	rVV2	163	251	0.02%	0.003%
36	6.245	1528	1541	1564	rBV	170977	331780	22.84%	4.239%

LSC Area Percent Report

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Sample : P2873-03 200X
Misc : 2.64g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0SG7

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\SFAMULM052924WMA.M
Title : VOC Analysis

37	6.534	1620	1631	1642	rVB6	3938	8185	0.56%	0.105%
38	6.579	1642	1645	1648	rBV	281	190	0.01%	0.002%
39	6.618	1654	1657	1660	rBV2	194	148	0.01%	0.002%
40	6.685	1665	1678	1703	rVV	108260	212951	14.66%	2.721%
41	6.898	1737	1744	1747	rBV2	319	405	0.03%	0.005%
42	6.959	1760	1763	1765	rBV	185	158	0.01%	0.002%
43	7.068	1794	1797	1800	rBV	244	170	0.01%	0.002%
44	7.100	1805	1807	1810	rBV	161	114	0.01%	0.001%
45	7.132	1814	1817	1819	rBV2	231	177	0.01%	0.002%
46	7.190	1830	1835	1843	rBV3	1355	1709	0.12%	0.022%
47	7.341	1878	1882	1883	rBV	224	154	0.01%	0.002%
48	7.380	1891	1894	1895	rBV	188	107	0.01%	0.001%
49	7.515	1933	1936	1939	rBV	188	176	0.01%	0.002%
50	7.563	1939	1951	1974	rVV2	46888	85905	5.91%	1.098%
51	7.753	2005	2010	2013	rBV	332	297	0.02%	0.004%
52	7.779	2015	2018	2021	rVV	224	163	0.01%	0.002%
53	7.798	2022	2024	2027	rVB2	299	146	0.01%	0.002%
54	7.894	2041	2054	2068	rBV	179504	311478	21.44%	3.980%
55	8.177	2132	2142	2163	rBV	32239	56294	3.88%	0.719%
56	8.367	2196	2201	2205	rBV	461	398	0.03%	0.005%
57	8.396	2205	2210	2213	rBV2	213	243	0.02%	0.003%
58	8.547	2243	2257	2273	rBV	742599	1256092	86.47%	16.050%
59	8.628	2274	2282	2317	rVB	125268	249463	17.17%	3.188%
60	9.078	2419	2422	2427	rBV2	274	304	0.02%	0.004%
61	9.226	2462	2468	2473	rBV	303	352	0.02%	0.004%
62	9.255	2474	2477	2480	rBV2	226	189	0.01%	0.002%
63	9.412	2514	2526	2554	rBV	248980	424906	29.25%	5.429%
64	9.566	2564	2574	2590	rBV	77327	122433	8.43%	1.564%
65	9.689	2601	2612	2634	rVB	75501	131076	9.02%	1.675%
66	9.824	2648	2654	2657	rBV2	420	434	0.03%	0.006%
67	9.920	2681	2684	2687	rBV2	297	236	0.02%	0.003%
68	10.033	2715	2719	2721	rBV2	257	196	0.01%	0.003%
69	10.100	2729	2740	2766	rVB4	35660	74146	5.10%	0.947%
70	10.193	2767	2769	2772	rVB2	256	107	0.01%	0.001%
71	10.277	2792	2795	2796	rBV	302	156	0.01%	0.002%
72	10.328	2809	2811	2815	rBV	230	182	0.01%	0.002%
73	10.422	2837	2840	2841	rBV	174	93	0.01%	0.001%
74	10.750	2930	2942	2961	rBV	165858	266852	18.37%	3.410%
75	10.907	2982	2991	3000	rBV3	2508	4230	0.29%	0.054%
76	10.997	3010	3019	3023	rBV2	10934	17154	1.18%	0.219%

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Sample : P2873-03 200X
Misc : 2.64g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0SG7

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\SFAMULM052924WMA.M
Title : VOC Analysis

77	11.087	3039	3047	3063	rVB2	12008	19580	1.35%	0.250%
78	11.319	3104	3119	3128	rBV6	6308	13273	0.91%	0.170%
79	11.463	3151	3164	3176	rBV3	38360	62175	4.28%	0.794%
80	11.534	3176	3186	3196	rBV2	48504	76454	5.26%	0.977%
81	11.737	3242	3249	3259	rBV5	992	1538	0.11%	0.020%
82	11.807	3259	3271	3289	rBV	257684	418391	28.80%	5.346%
83	11.949	3308	3315	3330	rVB3	6026	9425	0.65%	0.120%
84	12.090	3350	3359	3368	rBV4	8505	13263	0.91%	0.169%
85	12.190	3378	3390	3409	rBV	193907	320689	22.08%	4.098%
86	12.309	3416	3427	3446	rBV	116907	193854	13.35%	2.477%
87	12.750	3556	3564	3576	rVB3	10127	15237	1.05%	0.195%
88	13.026	3641	3650	3653	rBV4	4501	5951	0.41%	0.076%
89	13.155	3683	3690	3701	rVB7	5862	8883	0.61%	0.114%
90	13.296	3727	3734	3738	rBV5	1781	2050	0.14%	0.026%
91	13.518	3794	3803	3818	rVB2	18405	28981	2.00%	0.370%
92	13.624	3827	3836	3850	rVB3	20455	35506	2.44%	0.454%
93	13.814	3892	3895	3896	rBV	391	269	0.02%	0.003%
94	14.081	3966	3978	4007	rBV	919976	1452598	100.00%	18.561%
95	14.203	4009	4016	4029	rVB	12078	21842	1.50%	0.279%
96	14.479	4099	4102	4104	rBV2	618	491	0.03%	0.006%
97	14.676	4156	4163	4172	rBV6	2823	4338	0.30%	0.055%
98	15.219	4321	4332	4352	rBV	166719	278990	19.21%	3.565%
99	15.405	4380	4390	4406	rBV	108982	181394	12.49%	2.318%
100	15.955	4554	4561	4574	rVB2	6817	11369	0.78%	0.145%

Sum of corrected areas: 7825938

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
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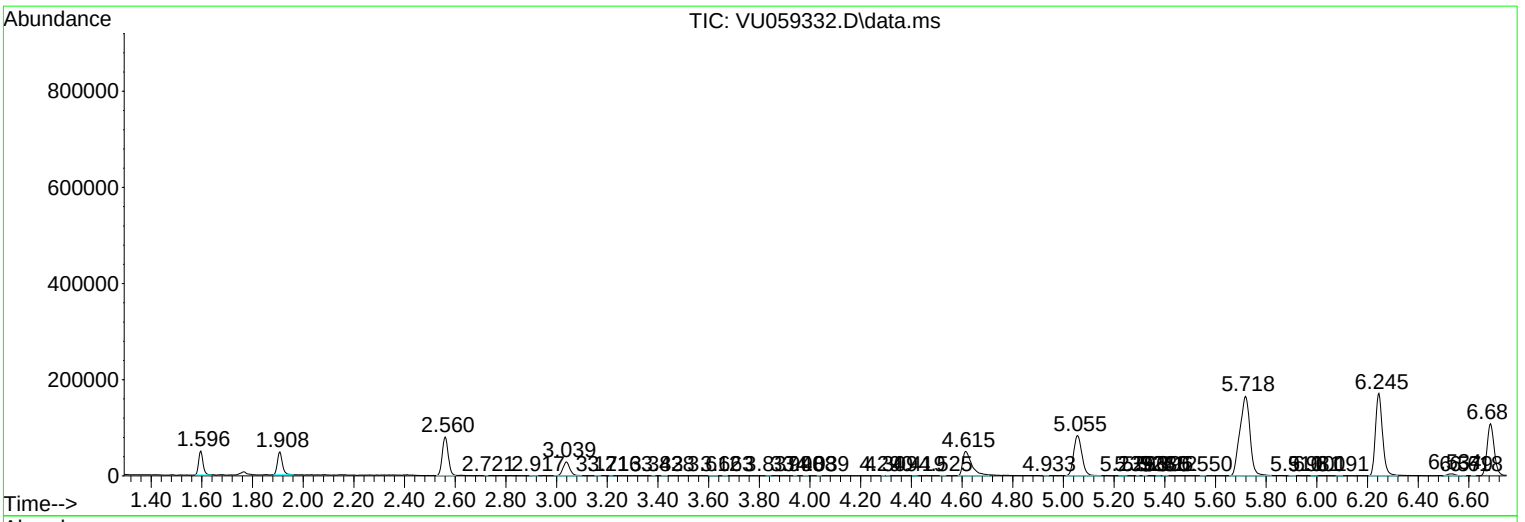
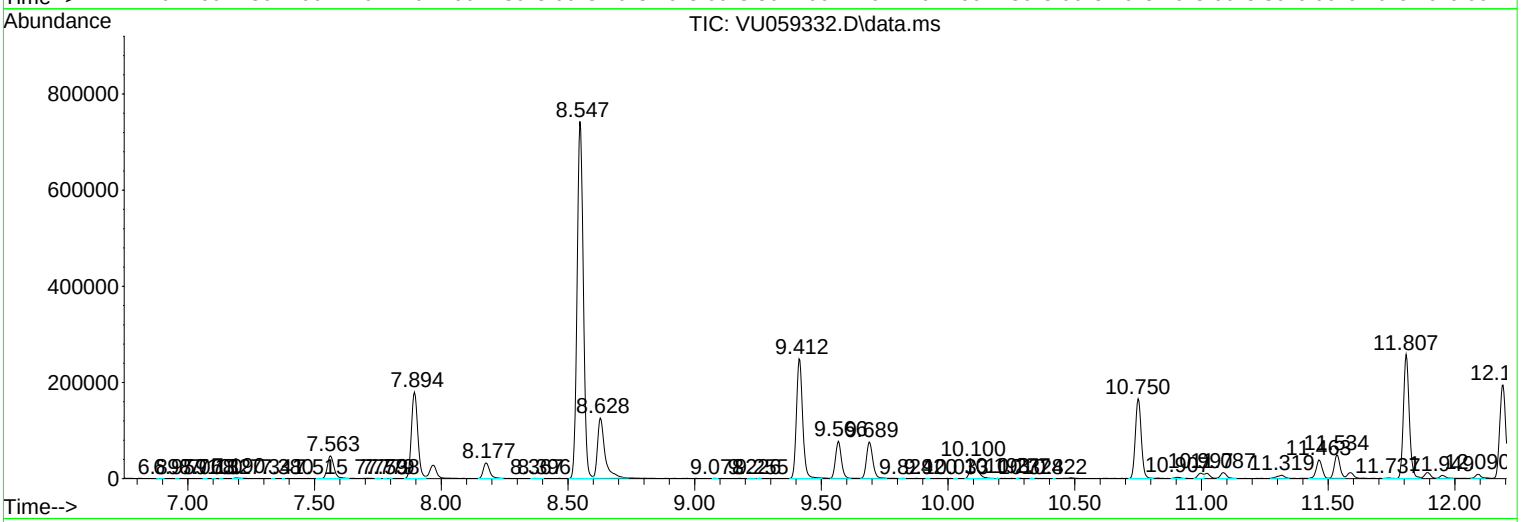
Sample : P2873-03 200X
Misc : 2.64g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 40 Sample Multiplier: 1

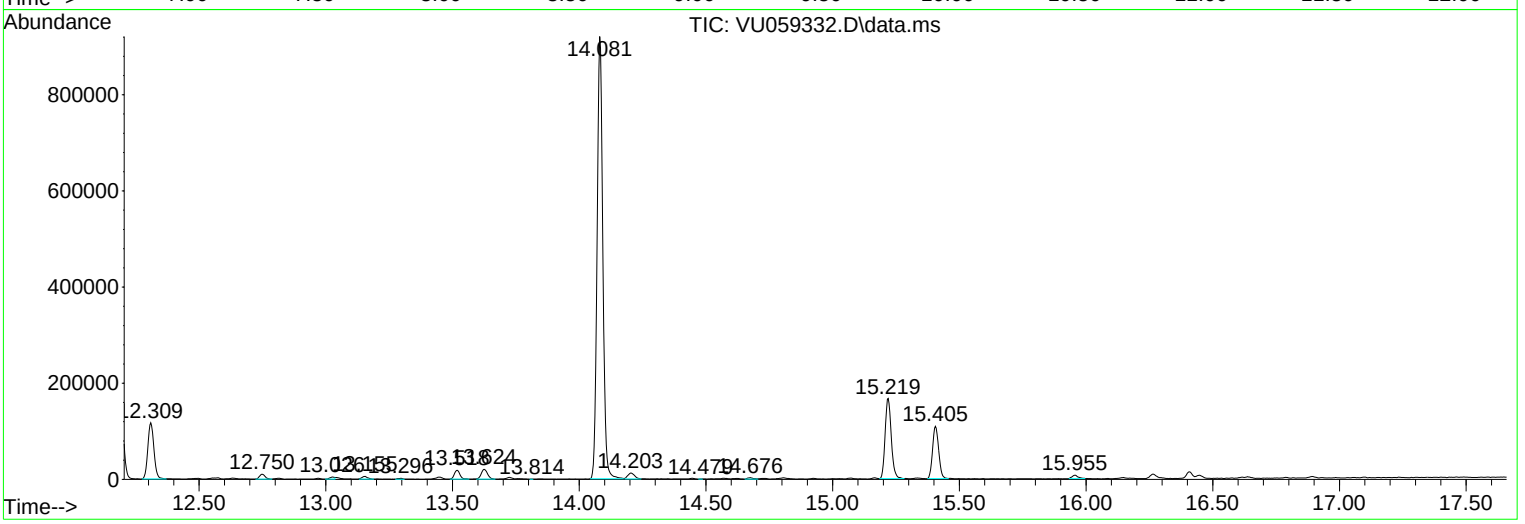
Instrument :
MSVOA_U
ClientSampleId :
C0SG7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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







Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
Data File : VU059332.D
Acq On : 18 Jun 2024 23:25
Operator : MD/SY
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Misc : 2.64g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0SG7

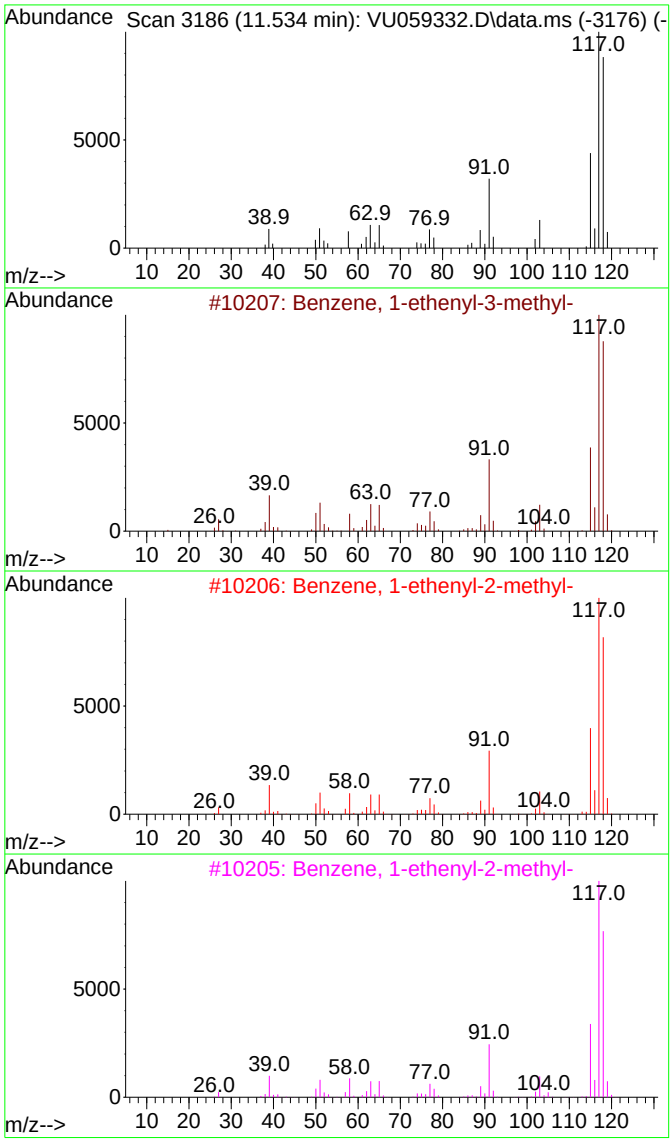
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

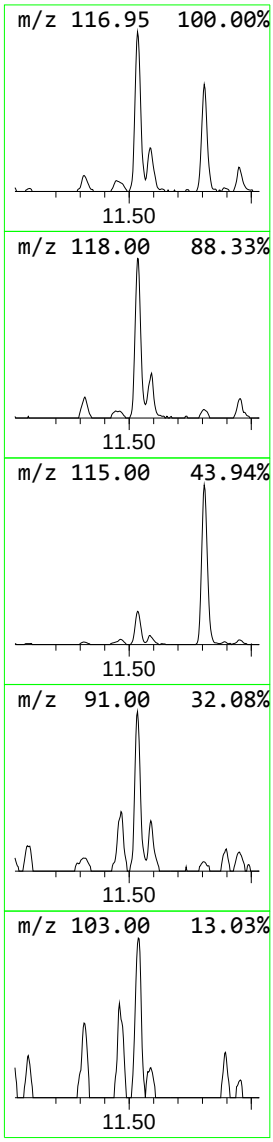
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzene, 1-ethenyl-3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.534	9.14 ug/L	76454	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	96
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	94
3	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	94
4	Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	94
5	Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
Data File : VU059332.D
Acq On : 18 Jun 2024 23:25
Operator : MD/SY
Sample : P2873-03 200X
Misc : 2.64g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0SG7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

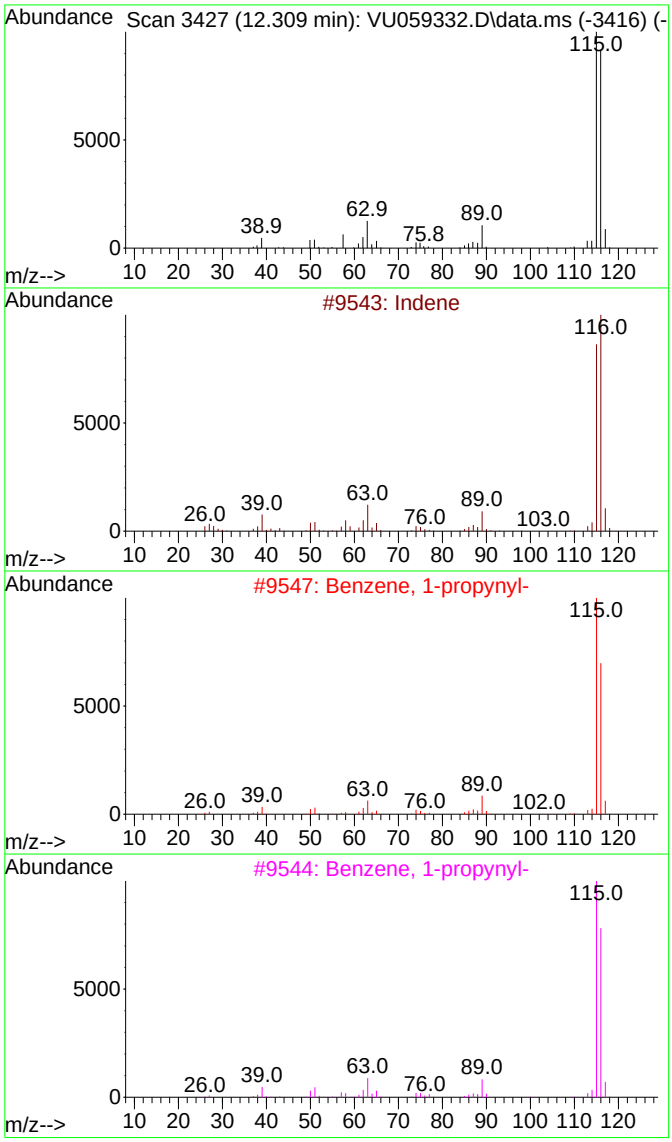
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

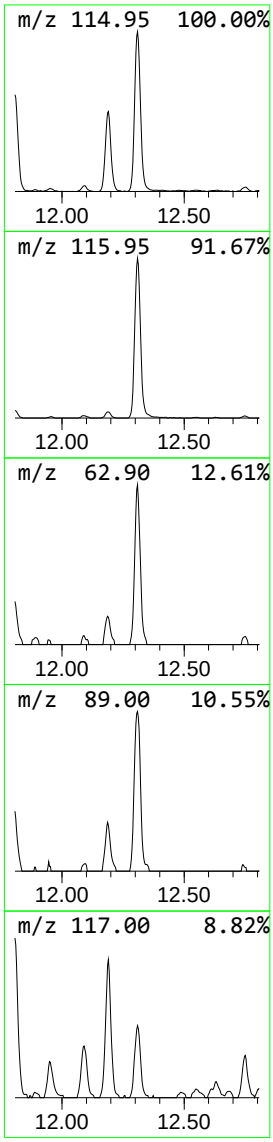
****

Peak Number 3 Indene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.309	23.17 ug/L	193854	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	95
2	Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
3	Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
4	1-Propyne, 3-phenyl-	116	C9H8	010147-11-2	91
5	Benzene, 1-propynyl-	116	C9H8	000673-32-5	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
Data File : VU059332.D
Acq On : 18 Jun 2024 23:25
Operator : MD/SY
Sample : P2873-03 200X
Misc : 2.64g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0SG7

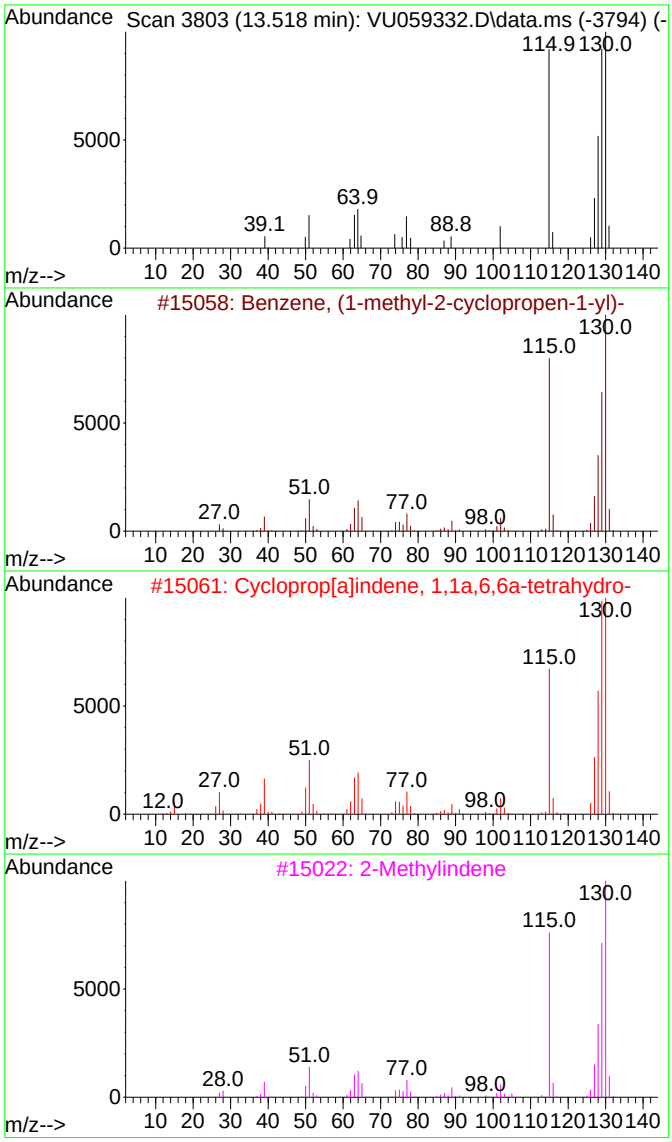
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

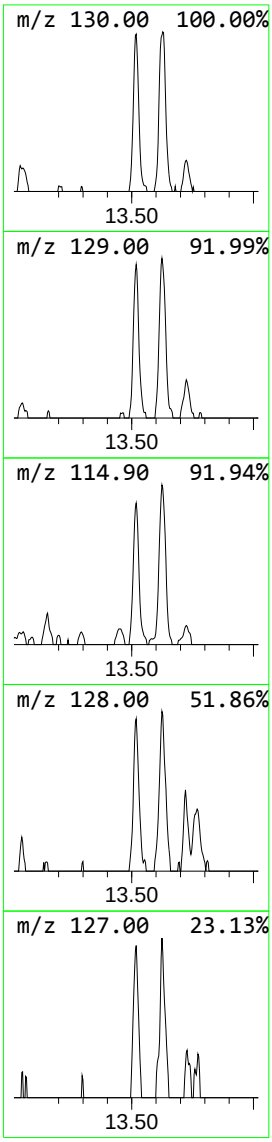
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, (1-methyl-2-cyclop... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.518	3.46 ug/L	28981	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	95
2	Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	95
3	2-Methylindene	130	C10H10	002177-47-1	94
4	Naphthalene, 1,2-dihydro-	130	C10H10	000447-53-0	93
5	1,4-Dihydronaphthalene	130	C10H10	000612-17-9	92





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
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Misc : 2.64g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0SG7

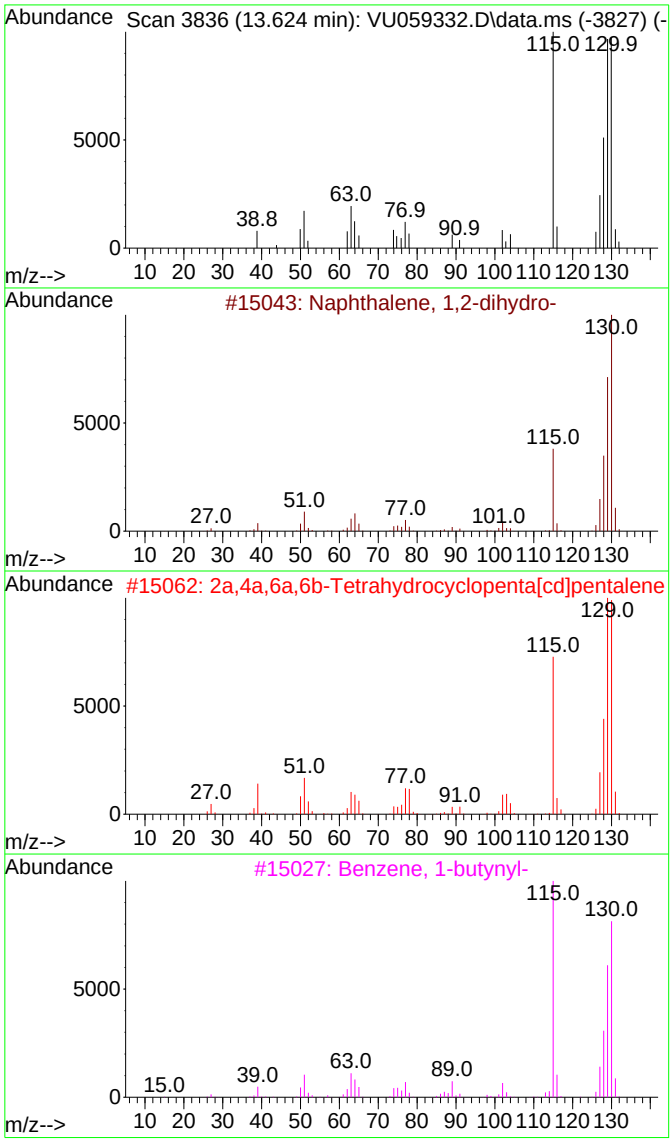
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

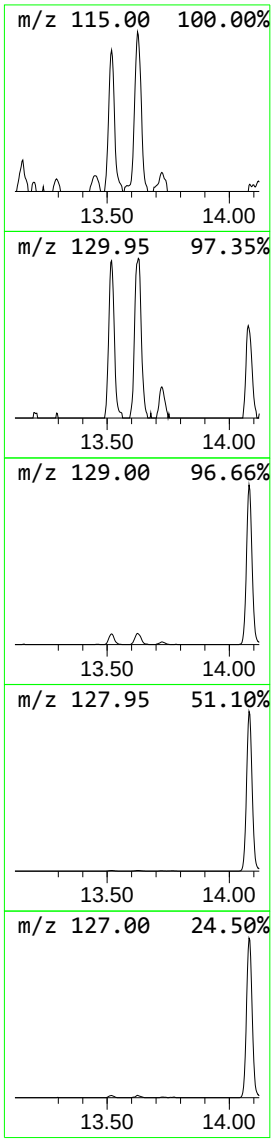
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Naphthalene, 1,2-dihydro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.624	4.24 ug/L	35506	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2-dihydro-	130	C10H10	000447-53-0	90
2	2a,4a,6a,6b-Tetrahydrocyclopenta...	130	C10H10	006053-74-3	90
3	Benzene, 1-butynyl-	130	C10H10	000622-76-4	81
4	Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	76
5	Tetracyclo[5.3.0.0<2,6>.0<3,10>]...	130	C10H10	034324-40-8	76





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
Data File : VU059332.D
Acq On : 18 Jun 2024 23:25
Operator : MD/SY
Sample : P2873-03 200X
Misc : 2.64g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0SG7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

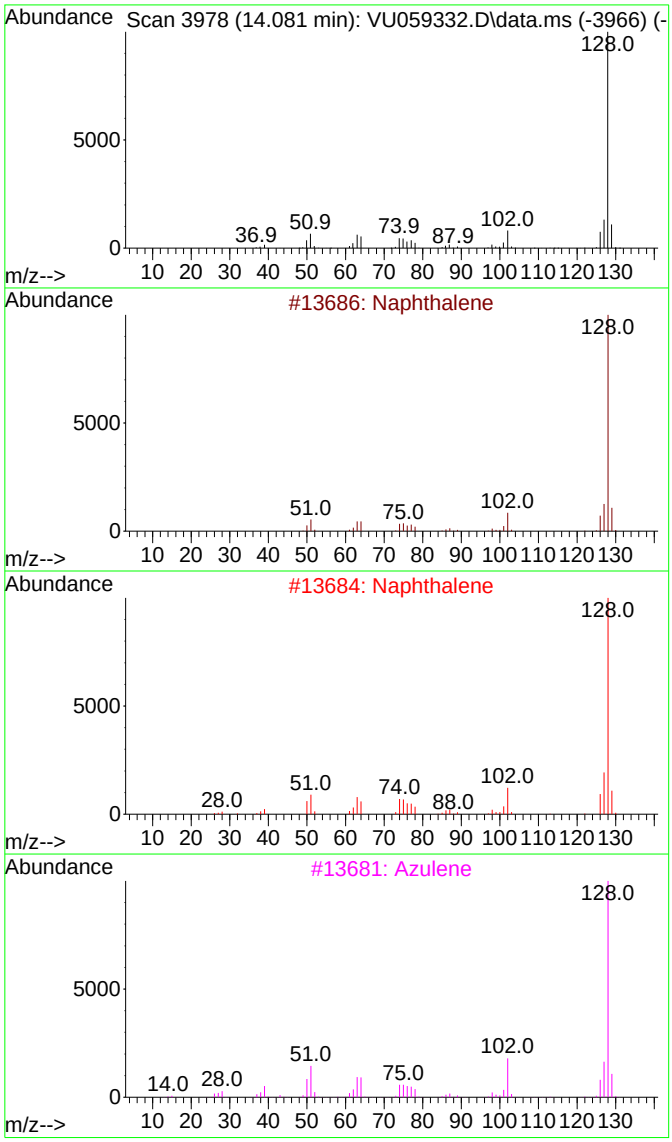
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

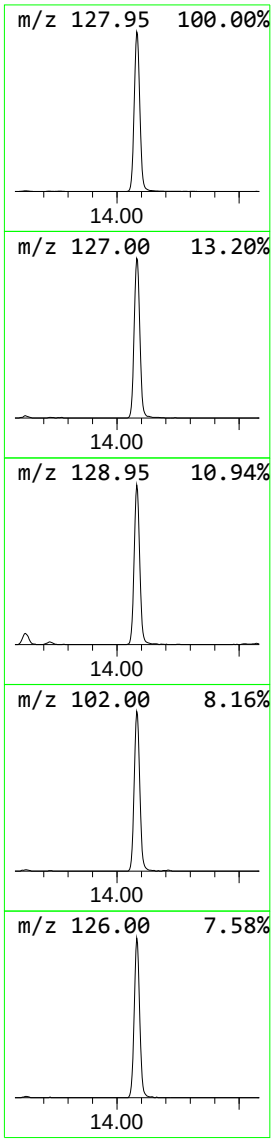
****

Peak Number 6 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.081	173.59 ug/L	1452600	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	Azulene	128	C10H8	000275-51-4	91
4	Azulene	128	C10H8	000275-51-4	91
5	Azulene	128	C10H8	000275-51-4	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
Data File : VU059332.D
Acq On : 18 Jun 2024 23:25
Operator : MD/SY
Sample : P2873-03 200X
Misc : 2.64g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0SG7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

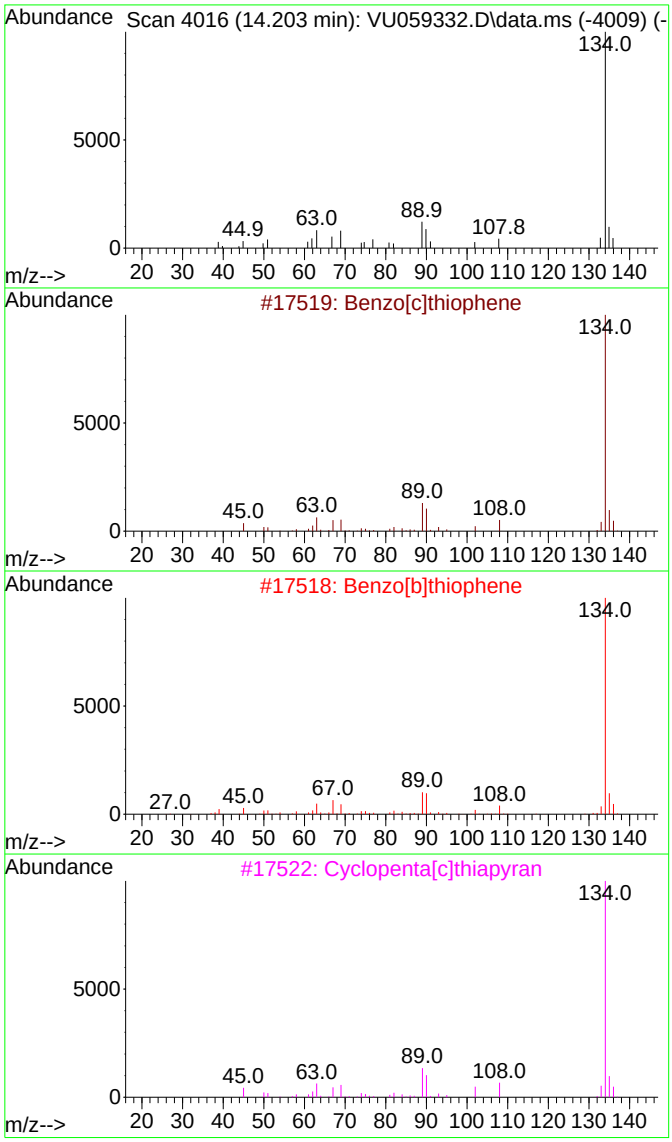
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

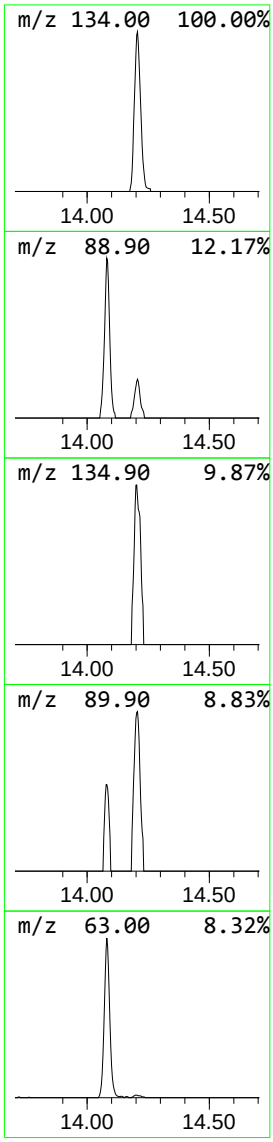
****

Peak Number 7 Benzo[c]thiophene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.203	2.61 ug/L	21842	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[c]thiophene	134	C8H6S	000270-82-6	94
2	Benzo[b]thiophene	134	C8H6S	000095-15-8	91
3	Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	87
4	Benzo[b]thiophene	134	C8H6S	000095-15-8	86
5	3-Deazaadenine	134	C6H6N4	006811-77-4	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
Data File : VU059332.D
Acq On : 18 Jun 2024 23:25
Operator : MD/SY
Sample : P2873-03 200X
Misc : 2.64g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0SG7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.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-ethe...	11.534	9.1	ug/L	76454	3	11.807	418391	50.0
Indene	12.309	23.2	ug/L	193854	3	11.807	418391	50.0
Benzene, (1-met...	13.518	3.5	ug/L	28981	3	11.807	418391	50.0
Naphthalene, 1,...	13.624	4.2	ug/L	35506	3	11.807	418391	50.0
Azulene	14.081	173.6	ug/L	1452600	3	11.807	418391	50.0
Benzo[c]thiophene	14.203	2.6	ug/L	21842	3	11.807	418391	50.0