LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
Data File : VX042767.D
Acq On : 31 Jul 2024 12:53
Operator : JC/MD
Sample : P3361-01ME
Misc : 11.96g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : E20N3ME

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_X\Method\SFAMXLM072624WMA.M
Title : VOC Analysis

Signal : TIC: VX042767.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	39	rVB2	16512	32822	8.98%	0.907%
2	1.368	43	46	48	rBV	7446	9320	2.55%	0.257%
3	2.270	188	194	203	rBV	47366	87961	24.07%	2.430%
4	2.538	236	238	241	rVB	135	142	0.04%	0.004%
5	2.569	241	243	244	rBV	202	170	0.05%	0.005%
6	2.636	250	254	257	rBV	299	495	0.14%	0.014%
7	2.697	261	264	265	rBV	140	135	0.04%	0.004%
8	2.709	265	266	268	rVB	266	130	0.04%	0.004%
9	2.776	269	277	282	rBV2	1954	4513	1.23%	0.125%
10	2.947	297	305	318	rBB	3291	8367	2.29%	0.231%
11	3.038	318	320	324	rBV	136	190	0.05%	0.005%
12	3.075	324	326	328	rVB	257	166	0.05%	0.005%
13	3.136	333	336	340	rBV2	147	274	0.07%	0.008%
14	3.416	379	382	386	rBB2	311	445	0.12%	0.012%
15	4.068	486	489	490	rBB2	174	132	0.04%	0.004%
16	4.434	547	549	551	rBB2	178	130	0.04%	0.004%
17	4.495	551	559	575	rBV	19690	66322	18.15%	1.832%
18	4.861	618	619	621	rVB	286	150	0.04%	0.004%
19	4.897	622	625	628	rBV	226	285	0.08%	0.008%
20	5.050	639	650	664	rBV2	45427	143641	39.30%	3.968%
21	5.324	693	695	698	rBB2	142	123	0.03%	0.003%
22	5.379	702	704	705	rBV2	218	141	0.04%	0.004%
23	5.477	719	720	726	rBB2	91	147	0.04%	0.004%
24	5.531	727	729	731	rBV2	281	344	0.09%	0.010%
25	5.745	761	764	768	rBB	201	226	0.06%	0.006%
26	5.964	789	800	815	rBV3	126540	360495	98.64%	9.959%
27	6.318	856	858	861	rBB3	194	192	0.05%	0.005%
28	6.367	861	866	867	rBV	902	951	0.26%	0.026%
29	6.757	922	930	944	rBV	115184	276802	75.74%	7.647%
30	7.062	977	980	981	rBV	173	163	0.04%	0.005%
31	7.123	981	990	1001	rBV	164293	365456	100.00%	10.096%
32	7.306	1013	1020	1038	rVB2	70677	159079	43.53%	4.395%
33	7.434	1038	1041	1043	rBV2	136	187	0.05%	0.005%
34	7.482	1047	1049	1054	rBB	181	240	0.07%	0.007%
35	7.525	1054	1056	1058	rBV2	218	237	0.06%	0.007%
36	7.696	1082	1084	1086	rBB2	208	184	0.05%	0.005%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
Data File : VX042767.D
Acq On : 31 Jul 2024 12:53
Operator : JC/MD
Sample : P3361-01ME
Misc : 11.96g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20N3ME

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_X\Method\SFAMXLM072624WMA.M
Title : VOC Analysis

37	7.787	1096	1099	1100	rBB2	272	169	0.05%	0.005%
38	7.854	1107	1110	1112	rBB	155	161	0.04%	0.004%
39	7.976	1124	1130	1133	rBB2	588	759	0.21%	0.021%
40	8.098	1147	1150	1151	rBV	128	135	0.04%	0.004%
41	8.141	1156	1157	1162	rBB	166	165	0.05%	0.005%
42	8.238	1172	1173	1175	rBV	142	124	0.03%	0.003%
43	8.257	1175	1176	1178	rBV	217	159	0.04%	0.004%
44	8.324	1182	1187	1202	rBV	43399	76068	20.81%	2.102%
45	8.482	1212	1213	1216	rBB	208	159	0.04%	0.004%
46	8.561	1222	1226	1228	rBB	121	159	0.04%	0.004%
47	8.647	1232	1240	1256	rBV	184352	303967	83.17%	8.398%
48	8.952	1285	1290	1305	rVV	30729	48927	13.39%	1.352%
49	9.049	1305	1306	1308	rVB	301	129	0.04%	0.004%
50	9.092	1309	1313	1314	rBV	140	183	0.05%	0.005%
51	9.281	1338	1344	1346	rBB	572	534	0.15%	0.015%
52	9.330	1349	1352	1353	rBB	130	124	0.03%	0.003%
53	9.397	1357	1363	1375	rBV	71316	152412	41.70%	4.211%
54	9.592	1394	1395	1398	rBV	276	308	0.08%	0.009%
55	9.634	1401	1402	1404	rBV	306	231	0.06%	0.006%
56	9.720	1411	1416	1423	rVB3	925	1764	0.48%	0.049%
57	9.787	1424	1427	1431	rBB2	197	301	0.08%	0.008%
58	9.951	1452	1454	1459	rBB2	146	199	0.05%	0.005%
59	9.994	1460	1461	1465	rBB2	156	149	0.04%	0.004%
60	10.055	1465	1471	1485	rBV	228976	327674	89.66%	9.053%
61	10.305	1508	1512	1517	rBB	764	980	0.27%	0.027%
62	10.646	1565	1568	1570	rBV2	318	378	0.10%	0.010%
63	10.756	1584	1586	1588	rBB2	144	124	0.03%	0.003%
64	10.860	1600	1603	1604	rBV2	156	146	0.04%	0.004%
65	10.909	1608	1611	1613	rBB2	155	165	0.05%	0.005%
66	10.963	1617	1620	1623	rBV	415	399	0.11%	0.011%
67	11.024	1626	1630	1632	rBB	163	219	0.06%	0.006%
68	11.195	1653	1658	1667	rVB	141480	181230	49.59%	5.007%
69	11.457	1699	1701	1703	rBV	395	322	0.09%	0.009%
70	11.585	1718	1722	1723	rBV	141	163	0.04%	0.005%
71	11.634	1728	1730	1731	rBB	183	131	0.04%	0.004%
72	11.756	1746	1750	1753	rVB3	474	505	0.14%	0.014%
73	11.908	1772	1775	1778	rBV3	145	232	0.06%	0.006%
74	11.963	1782	1784	1788	rVB2	1077	971	0.27%	0.027%
75	12.024	1788	1794	1804	rBV	252425	318653	87.19%	8.803%
76	12.183	1818	1820	1825	rVB3	196	268	0.07%	0.007%

LSC Area Percent Report

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Acq On : 31 Jul 2024 12:53
Operator : JC/MD
Sample : P3361-01ME
Misc : 11.96g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20N3ME

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_X\Method\SFAMXLM072624WMA.M
Title : VOC Analysis

77	12.244	1825	1830	1835	rVB	4536	5821	1.59%	0.161%
78	12.323	1837	1843	1854	rBV	208329	275478	75.38%	7.611%
79	12.487	1866	1870	1873	rBV2	174	309	0.08%	0.009%
80	12.555	1878	1881	1882	rVB2	234	197	0.05%	0.005%
81	12.579	1883	1885	1886	rBV2	218	156	0.04%	0.004%
82	12.652	1894	1897	1898	rBB	132	133	0.04%	0.004%
83	12.701	1899	1905	1906	rBV2	423	592	0.16%	0.016%
84	13.774	2077	2081	2093	rVB	141092	188989	51.71%	5.221%
85	13.871	2093	2097	2102	rVB2	7506	9872	2.70%	0.273%
86	14.127	2130	2139	2148	rBV7	4502	14746	4.03%	0.407%
87	14.323	2169	2171	2173	rBV3	772	901	0.25%	0.025%
88	14.451	2190	2192	2198	rVB3	346	551	0.15%	0.015%
89	14.524	2202	2204	2208	rBV2	684	1044	0.29%	0.029%
90	14.640	2219	2223	2233	rVB	26992	37232	10.19%	1.029%
91	14.780	2242	2246	2252	rBV	15321	19532	5.34%	0.540%
92	14.902	2262	2266	2270	rBV5	1472	2671	0.73%	0.074%
93	15.207	2312	2316	2322	rBV2	5903	8618	2.36%	0.238%
94	15.377	2341	2344	2351	rVB5	1470	2700	0.74%	0.075%
95	15.609	2379	2382	2386	rBV4	2440	3511	0.96%	0.097%
96	15.780	2409	2410	2412	rBV	302	266	0.07%	0.007%
97	16.091	2457	2461	2467	rVB5	2049	3763	1.03%	0.104%
98	16.225	2481	2483	2484	rBV	321	245	0.07%	0.007%
99	16.328	2493	2500	2513	rVB2	18855	35300	9.66%	0.975%
100	16.688	2552	2559	2569	rBV	31969	66439	18.18%	1.835%

Sum of corrected areas: 3619669

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
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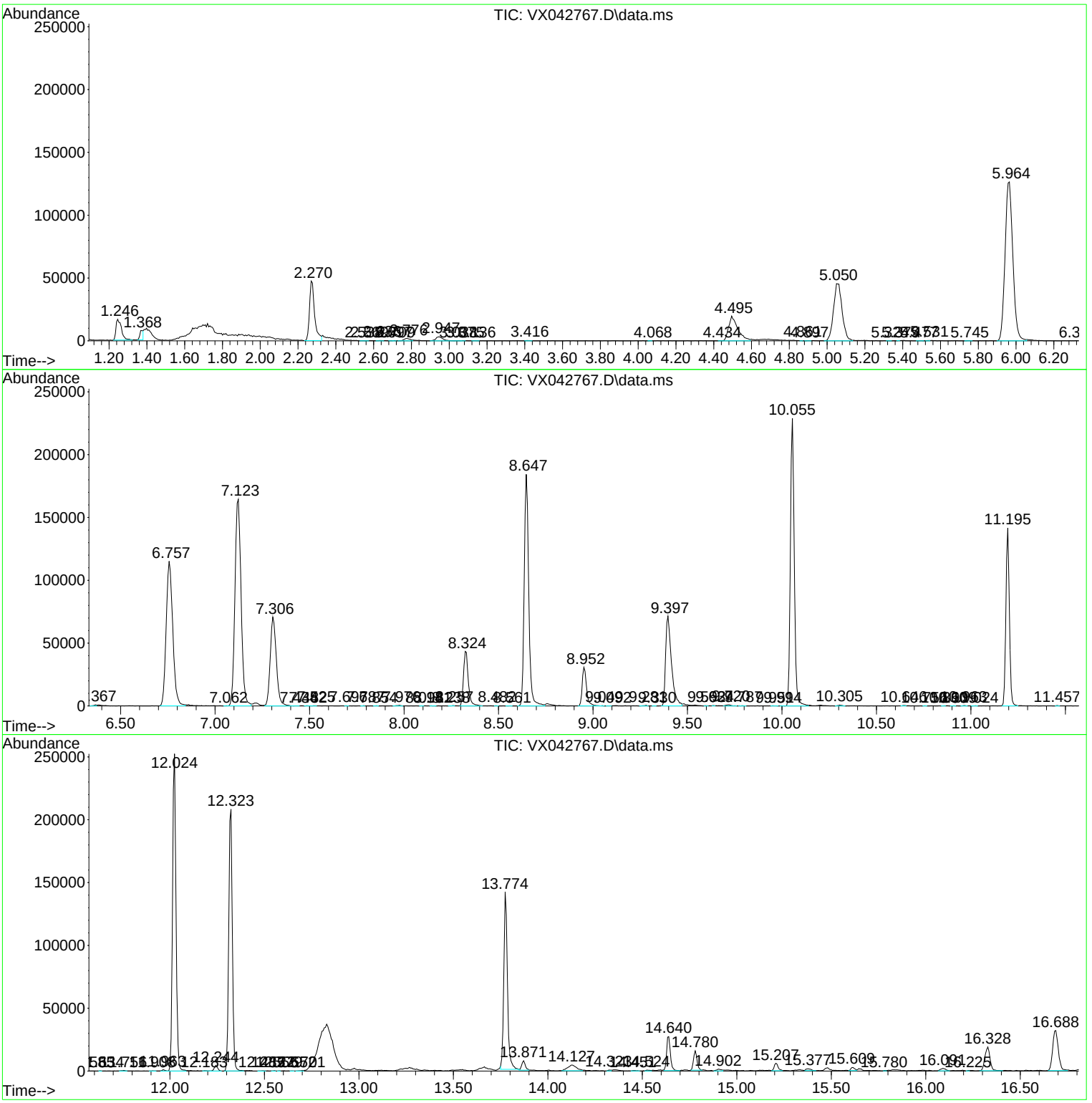
Operator : JC/MD
Sample : P3361-01ME
Misc : 11.96g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20N3ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM072624WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
Data File : VX042767.D
Acq On : 31 Jul 2024 12:53
Operator : JC/MD
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Misc : 11.96g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20N3ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM072624WMA.M
Quant Title : VOC Analysis

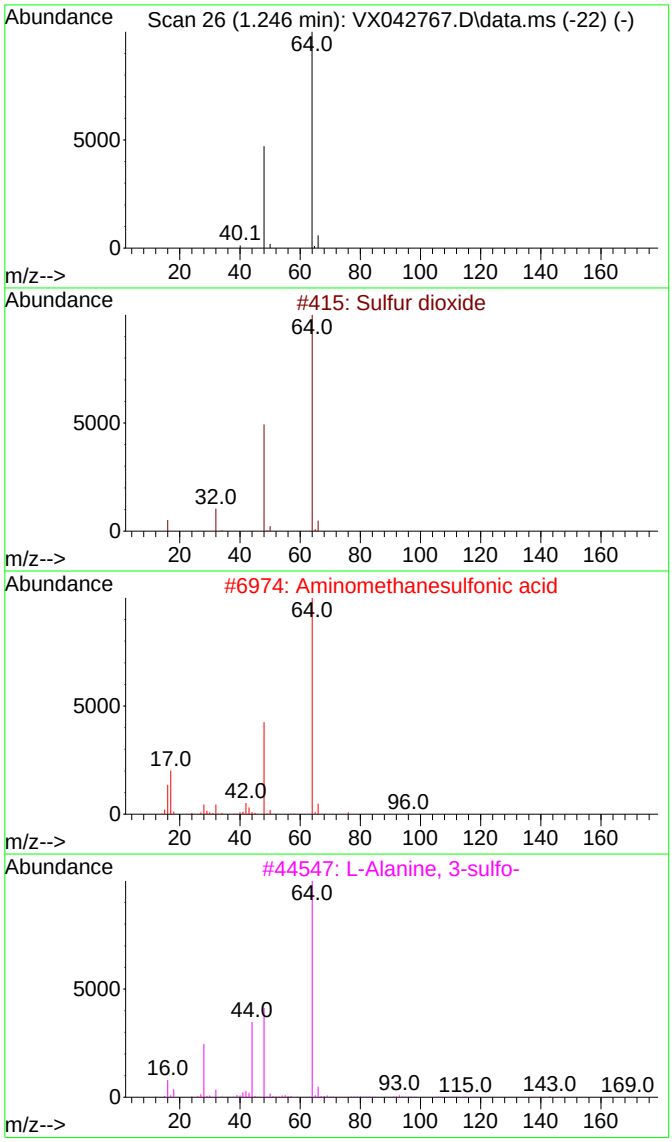
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

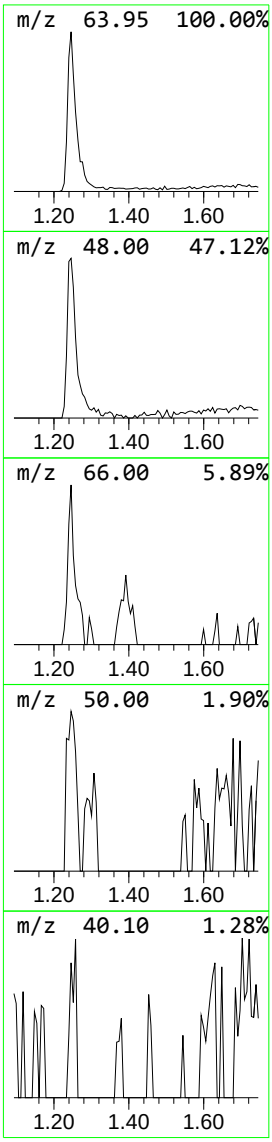
****

Peak Number 1 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	5.93 ug/L	32822	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	90
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Sulfur dioxide	64	O2S	007446-09-5	5
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
Data File : VX042767.D
Acq On : 31 Jul 2024 12:53
Operator : JC/MD
Sample : P3361-01ME
Misc : 11.96g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20N3ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM072624WMA.M
Quant Title : VOC Analysis

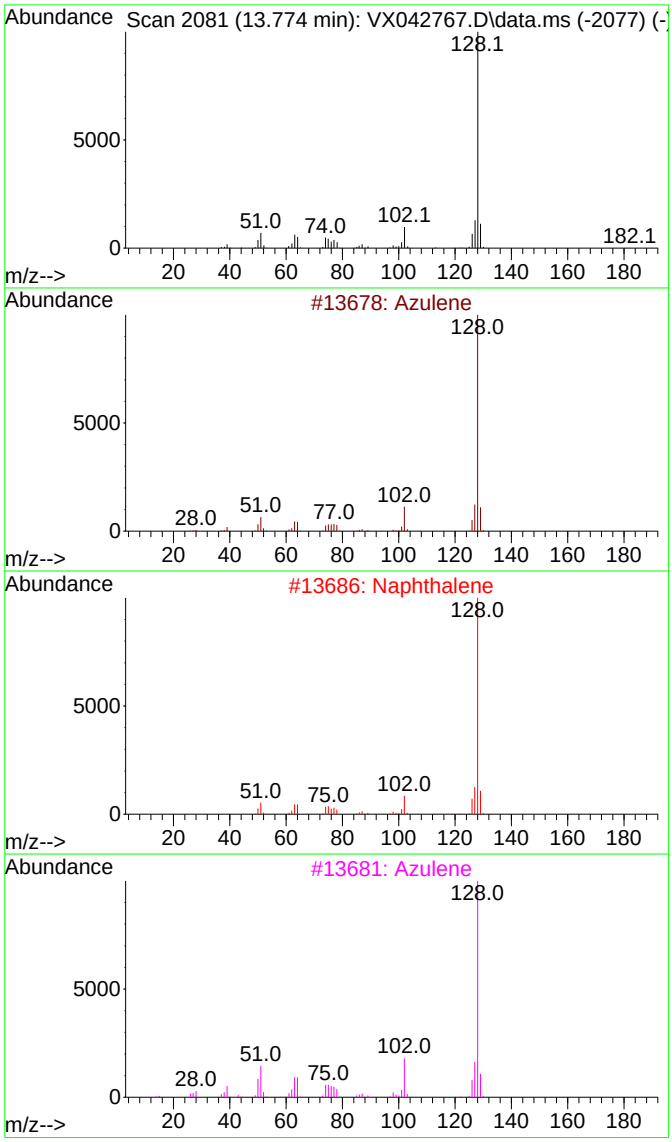
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

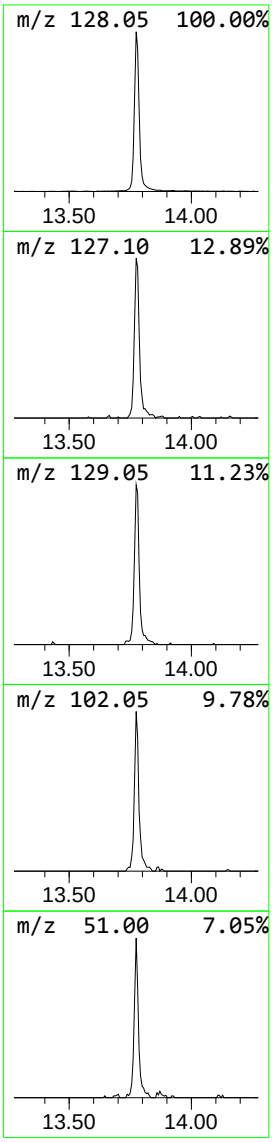
****

Peak Number 3 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	29.65 ug/L	188989	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Azulene	128	C10H8	000275-51-4	95
2	Naphthalene	128	C10H8	000091-20-3	95
3	Azulene	128	C10H8	000275-51-4	91
4	Naphthalene	128	C10H8	000091-20-3	91
5	Azulene	128	C10H8	000275-51-4	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
Data File : VX042767.D
Acq On : 31 Jul 2024 12:53
Operator : JC/MD
Sample : P3361-01ME
Misc : 11.96g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20N3ME

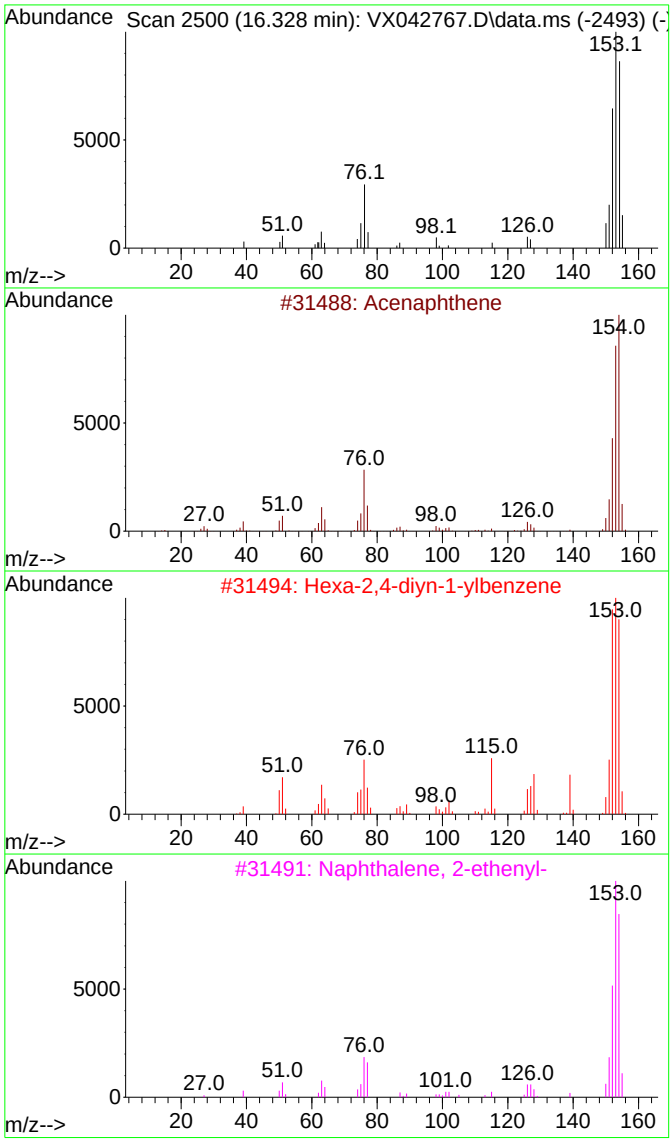
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM072624WMA.M
Quant Title : VOC Analysis

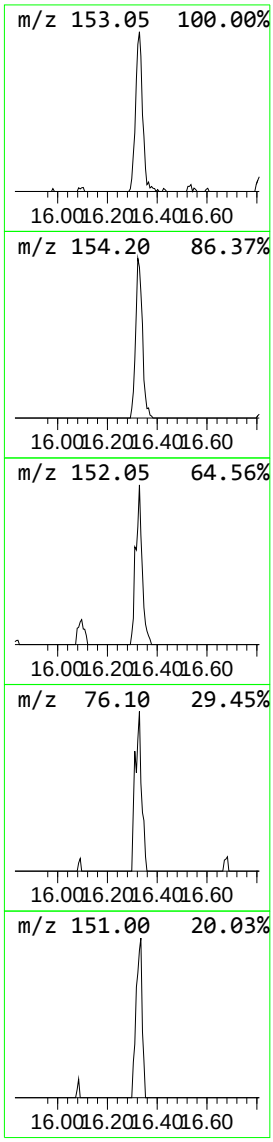
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Hexa-2,4-diyn-1-ylbenzene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.328	5.54 ug/L	35300	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acenaphthene	154	C12H10	000083-32-9	64
2	Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	64
3	Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	58
4	Acenaphthene	154	C12H10	000083-32-9	53
5	Acenaphthene	154	C12H10	000083-32-9	49





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
Data File : VX042767.D
Acq On : 31 Jul 2024 12:53
Operator : JC/MD
Sample : P3361-01ME
Misc : 11.96g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20N3ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM072624WMA.M
Quant Title : VOC Analysis

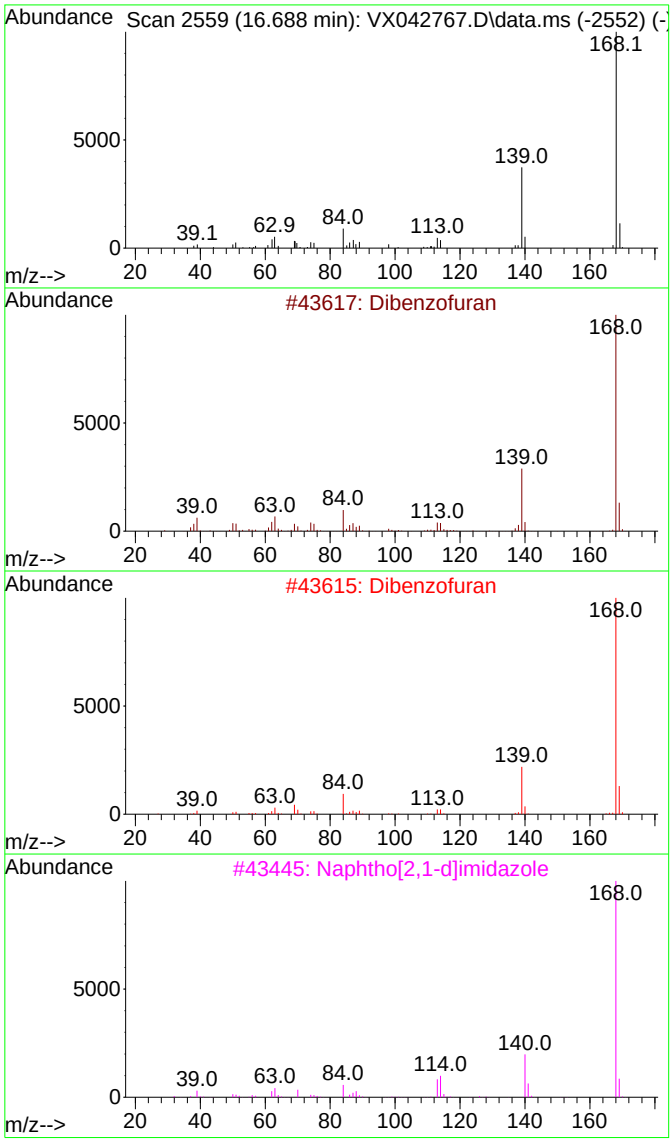
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

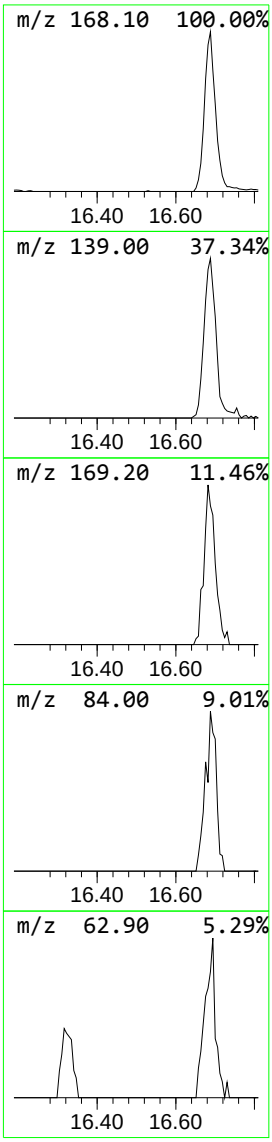
****

Peak Number 7 Naphtho[2,1-d]imidazole Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.688	10.43 ug/L	66439	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzofuran	168	C12H8O	000132-64-9	97
2	Dibenzofuran	168	C12H8O	000132-64-9	83
3	Naphtho[2,1-d]imidazole	168	C11H8N2	000233-53-4	64
4	9H-Pyrido[3,4-b]indole	168	C11H8N2	000244-63-3	64
5	9H-Pyrido[3,4-b]indole	168	C11H8N2	000244-63-3	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
Data File : VX042767.D
Acq On : 31 Jul 2024 12:53
Operator : JC/MD
Sample : P3361-01ME
Misc : 11.96g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20N3ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM072624WMA.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
Sulfur dioxide	1.246	5.9	ug/L	32822	1	6.757	276802	50.0
Azulene	13.774	29.6	ug/L	188989	3	12.024	318653	50.0
Hexa-2,4-diyn-1...	16.328	5.5	ug/L	35300	3	12.024	318653	50.0
Naphtho[2,1-d]i...	16.688	10.4	ug/L	66439	3	12.024	318653	50.0