LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
Data File : VX042768.D
Acq On : 31 Jul 2024 13:17
Operator : JC/MD
Sample : P3361-04ME
Misc : 10.82g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : E20N8ME

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: VX042768.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	33	rBV2	14051	28408	5.41%	0.746%
2	1.374	43	47	48	rBV	9727	11684	2.22%	0.307%
3	2.276	189	195	212	rBV	57563	108203	20.60%	2.840%
4	2.776	271	277	283	rBV3	1748	3389	0.65%	0.089%
5	2.947	297	305	314	rBV	4450	10180	1.94%	0.267%
6	3.038	317	320	322	rBB	187	150	0.03%	0.004%
7	3.075	322	326	329	rBB	297	335	0.06%	0.009%
8	3.148	333	338	340	rBB	145	203	0.04%	0.005%
9	3.215	346	349	351	rBB	187	171	0.03%	0.004%
10	3.684	423	426	429	rBV	160	233	0.04%	0.006%
11	3.824	446	449	451	rBB	146	142	0.03%	0.004%
12	4.081	487	491	494	rBB	146	243	0.05%	0.006%
13	4.148	501	502	504	rBV	167	142	0.03%	0.004%
14	4.489	551	558	570	rBV2	23691	76025	14.47%	1.996%
15	5.062	638	652	665	rVV2	53216	164737	31.36%	4.324%
16	5.312	691	693	696	rVV	173	178	0.03%	0.005%
17	5.379	702	704	707	rBV	295	253	0.05%	0.007%
18	5.410	707	709	711	rVB	217	141	0.03%	0.004%
19	5.538	728	730	731	rBV	348	302	0.06%	0.008%
20	5.641	746	747	750	rBB	213	165	0.03%	0.004%
21	5.818	773	776	778	rBV	122	176	0.03%	0.005%
22	5.964	790	800	816	rBV3	139601	403832	76.88%	10.600%
23	6.220	839	842	844	rBV3	139	217	0.04%	0.006%
24	6.336	858	861	862	rBV	161	215	0.04%	0.006%
25	6.476	883	884	887	rBV	146	144	0.03%	0.004%
26	6.757	920	930	948	rBV	112111	273047	51.98%	7.167%
27	7.013	967	972	977	rBB2	214	350	0.07%	0.009%
28	7.123	980	990	1003	rBV	234638	525255	100.00%	13.787%
29	7.306	1012	1020	1037	rVB	82712	185355	35.29%	4.865%
30	7.482	1047	1049	1054	rVB	328	316	0.06%	0.008%
31	7.543	1054	1059	1061	rBV2	202	354	0.07%	0.009%
32	7.604	1065	1069	1070	rBB2	118	159	0.03%	0.004%
33	7.751	1087	1093	1094	rVV2	165	205	0.04%	0.005%
34	7.854	1107	1110	1112	rBB2	146	147	0.03%	0.004%
35	7.946	1123	1125	1127	rBV2	136	143	0.03%	0.004%
36	7.970	1127	1129	1132	rBV2	239	262	0.05%	0.007%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
Data File : VX042768.D
Acq On : 31 Jul 2024 13:17
Operator : JC/MD
Sample : P3361-04ME
Misc : 10.82g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20N8ME

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	8.159	1159	1160	1163	rBV2	175	219	0.04%	0.006%
38	8.324	1180	1187	1196	rBV	49738	86962	16.56%	2.283%
39	8.494	1212	1215	1217	rBV	136	159	0.03%	0.004%
40	8.543	1221	1223	1226	rBV	167	218	0.04%	0.006%
41	8.647	1234	1240	1256	rBV	217104	351234	66.87%	9.219%
42	8.866	1274	1276	1278	rBB	304	268	0.05%	0.007%
43	8.915	1281	1284	1285	rBV	194	143	0.03%	0.004%
44	8.952	1285	1290	1303	rVV	36603	57650	10.98%	1.513%
45	9.104	1314	1315	1316	rBV	257	153	0.03%	0.004%
46	9.183	1324	1328	1330	rBV	119	193	0.04%	0.005%
47	9.269	1340	1342	1348	rVB	338	496	0.09%	0.013%
48	9.360	1354	1357	1358	rBV	217	255	0.05%	0.007%
49	9.397	1358	1363	1383	rBV	85194	183307	34.90%	4.812%
50	9.653	1401	1405	1406	rBV	290	301	0.06%	0.008%
51	9.708	1410	1414	1420	rBB3	1007	1527	0.29%	0.040%
52	9.817	1430	1432	1434	rBV	174	193	0.04%	0.005%
53	9.909	1446	1447	1450	rBV	227	178	0.03%	0.005%
54	10.000	1460	1462	1465	rVB	213	176	0.03%	0.005%
55	10.055	1465	1471	1486	rBV	230395	324174	61.72%	8.509%
56	10.256	1503	1504	1506	rBB	266	186	0.04%	0.005%
57	10.305	1509	1512	1517	rBV2	608	841	0.16%	0.022%
58	10.433	1531	1533	1537	rBB2	179	240	0.05%	0.006%
59	10.494	1542	1543	1546	rBV	151	184	0.04%	0.005%
60	10.549	1550	1552	1554	rBV	218	227	0.04%	0.006%
61	10.653	1562	1569	1571	rBV2	429	763	0.15%	0.020%
62	10.732	1579	1582	1586	rBB	110	177	0.03%	0.005%
63	10.768	1586	1588	1590	rBV	155	171	0.03%	0.004%
64	10.970	1616	1621	1625	rBB2	286	453	0.09%	0.012%
65	11.006	1626	1627	1632	rBB2	161	203	0.04%	0.005%
66	11.116	1643	1645	1648	rBV2	211	210	0.04%	0.006%
67	11.195	1652	1658	1667	rBV	159396	212367	40.43%	5.574%
68	11.567	1716	1719	1720	rBV	163	176	0.03%	0.005%
69	11.634	1727	1730	1731	rBV	145	141	0.03%	0.004%
70	11.658	1731	1734	1737	rVV	202	196	0.04%	0.005%
71	11.756	1747	1750	1754	rVB2	456	597	0.11%	0.016%
72	11.872	1767	1769	1771	rBV	136	145	0.03%	0.004%
73	11.927	1774	1778	1780	rBV	166	245	0.05%	0.006%
74	12.024	1789	1794	1807	rVB	233416	301459	57.39%	7.913%
75	12.164	1816	1817	1819	rBV	188	178	0.03%	0.005%
76	12.244	1826	1830	1835	rBV2	2472	3438	0.65%	0.090%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
Data File : VX042768.D
Acq On : 31 Jul 2024 13:17
Operator : JC/MD
Sample : P3361-04ME
Misc : 10.82g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20N8ME

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	12.323	1837	1843	1851	rBV	231672	305928	58.24%	8.030%
78	12.475	1865	1868	1870	rBV2	261	283	0.05%	0.007%
79	12.518	1873	1875	1878	rBV	229	230	0.04%	0.006%
80	12.555	1878	1881	1882	rVV	268	184	0.04%	0.005%
81	13.073	1964	1966	1968	rBV	224	213	0.04%	0.006%
82	13.134	1974	1976	1978	rVB	300	212	0.04%	0.006%
83	13.158	1978	1980	1981	rBV	359	243	0.05%	0.006%
84	13.219	1986	1990	1992	rBV3	537	679	0.13%	0.018%
85	13.335	2008	2009	2012	rBV	170	178	0.03%	0.005%
86	13.506	2036	2037	2038	rBV	383	178	0.03%	0.005%
87	13.585	2049	2050	2052	rBV	159	148	0.03%	0.004%
88	13.640	2054	2059	2060	rBV	640	871	0.17%	0.023%
89	13.774	2075	2081	2093	rBV	70313	102301	19.48%	2.685%
90	14.231	2155	2156	2158	rBV	266	150	0.03%	0.004%
91	14.341	2172	2174	2175	rBV	267	159	0.03%	0.004%
92	14.640	2218	2223	2228	rBV	11483	15164	2.89%	0.398%
93	14.780	2240	2246	2251	rBV	6208	8655	1.65%	0.227%
94	14.902	2264	2266	2267	rBV	416	392	0.07%	0.010%
95	15.207	2312	2316	2322	rBV3	2412	3642	0.69%	0.096%
96	15.572	2374	2376	2380	rBV3	579	656	0.12%	0.017%
97	16.091	2457	2461	2467	rBV5	817	1844	0.35%	0.048%
98	16.328	2493	2500	2506	rBV2	8572	15829	3.01%	0.415%
99	16.530	2531	2533	2536	rBV2	468	487	0.09%	0.013%
100	16.688	2553	2559	2567	rBV	13683	25272	4.81%	0.663%

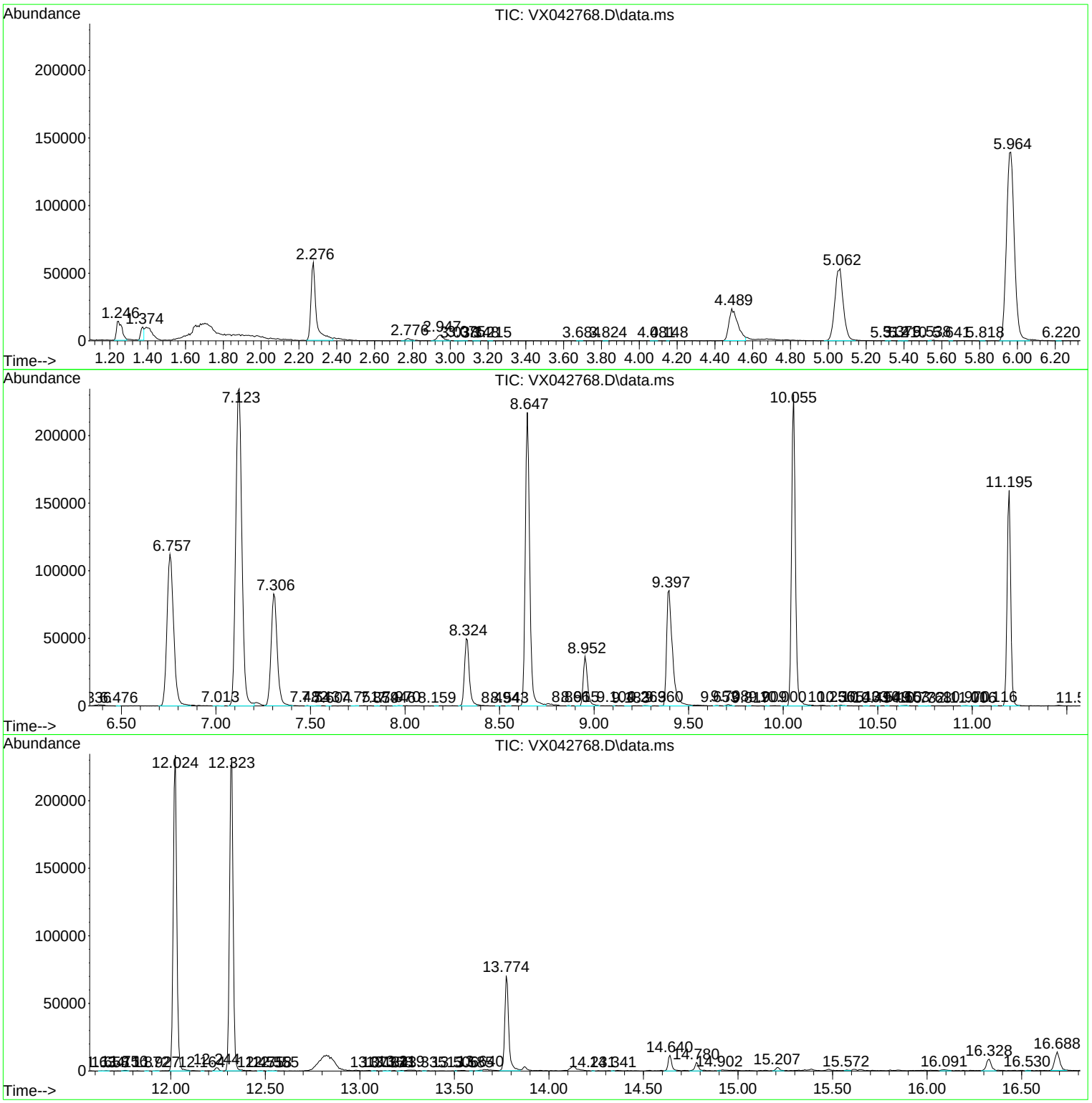
Sum of corrected areas: 3809762

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
Data File : VX042768.D
Acq On : 31 Jul 2024 13:17
Operator : JC/MD
Sample : P3361-04ME
Misc : 10.82g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20N8ME

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 : VX042768.D
Acq On : 31 Jul 2024 13:17
Operator : JC/MD
Sample : P3361-04ME
Misc : 10.82g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20N8ME

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

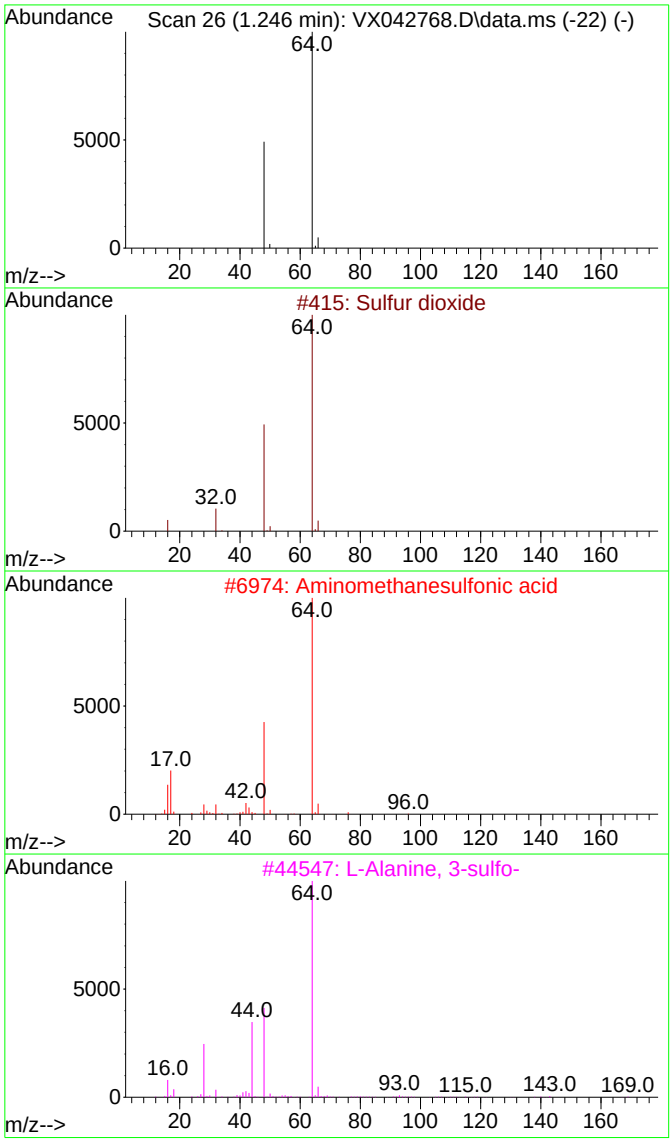
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

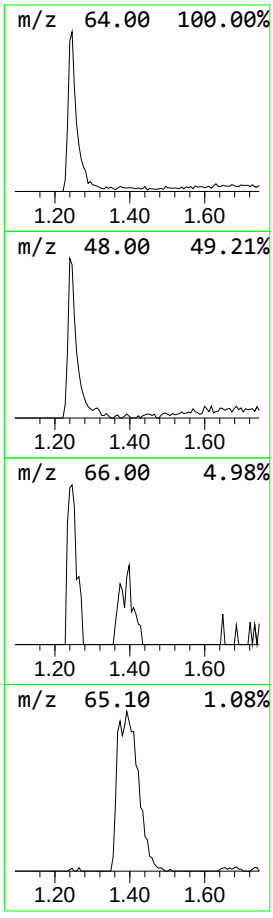
****

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	5.20 ug/L	28408	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	4
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
Data File : VX042768.D
Acq On : 31 Jul 2024 13:17
Operator : JC/MD
Sample : P3361-04ME
Misc : 10.82g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20N8ME

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

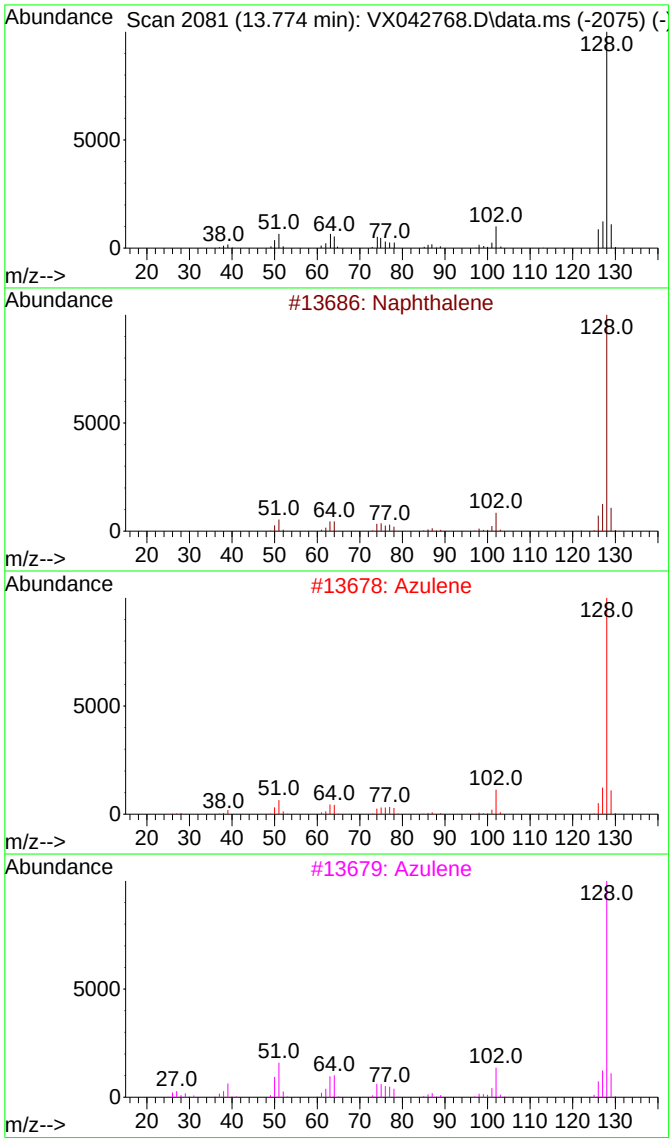
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

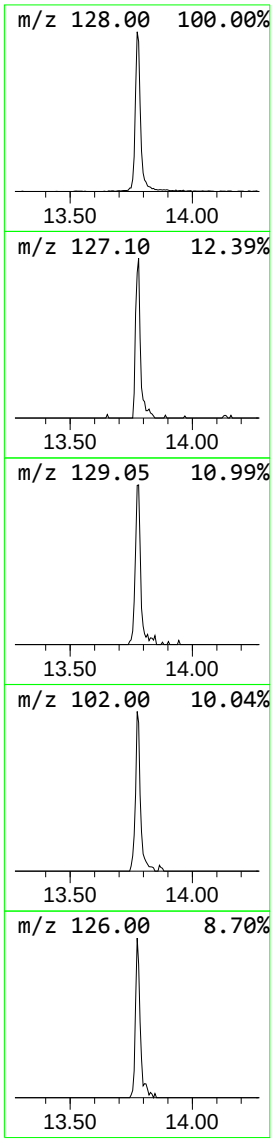
****

Peak Number 3 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	16.97 ug/L	102301	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene	128	C10H8	000091-20-3	95
2	Azulene	128	C10H8	000275-51-4	94
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 : VX042768.D
Acq On : 31 Jul 2024 13:17
Operator : JC/MD
Sample : P3361-04ME
Misc : 10.82g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20N8ME

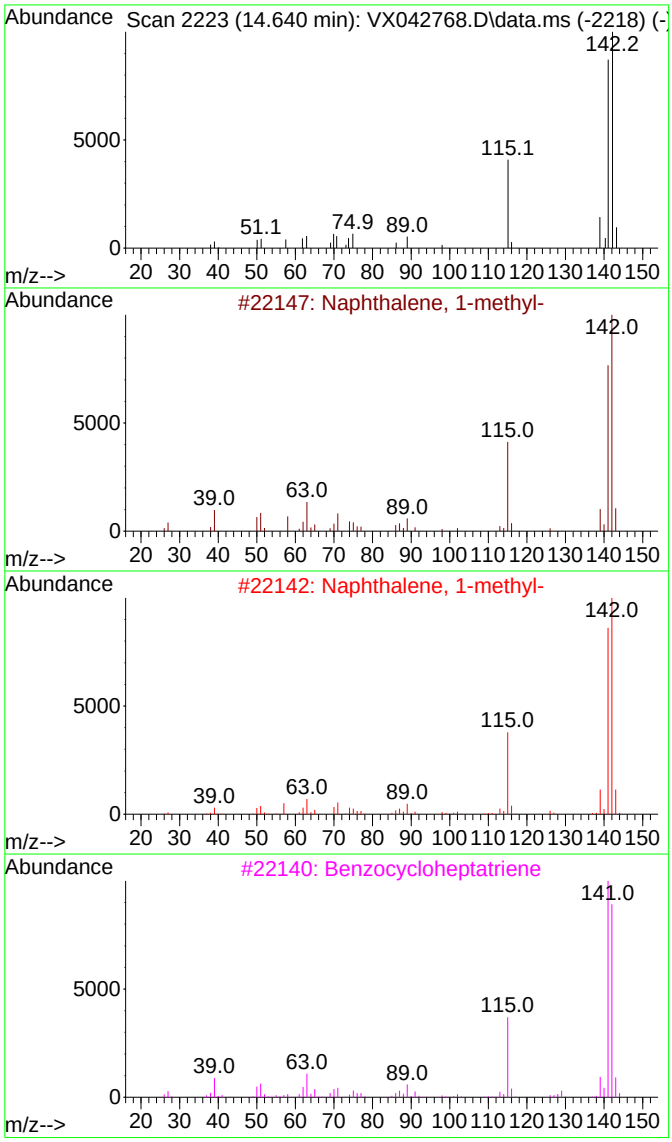
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM072624WMA.M
Quant Title : VOC Analysis

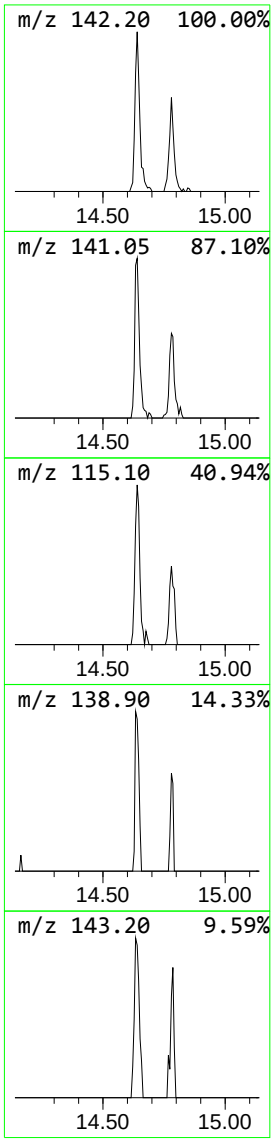
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzocycloheptatriene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	2.52 ug/L	15164	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91
3	Benzocycloheptatriene	142	C11H10	000264-09-5	91
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
5	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	86





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
Data File : VX042768.D
Acq On : 31 Jul 2024 13:17
Operator : JC/MD
Sample : P3361-04ME
Misc : 10.82g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20N8ME

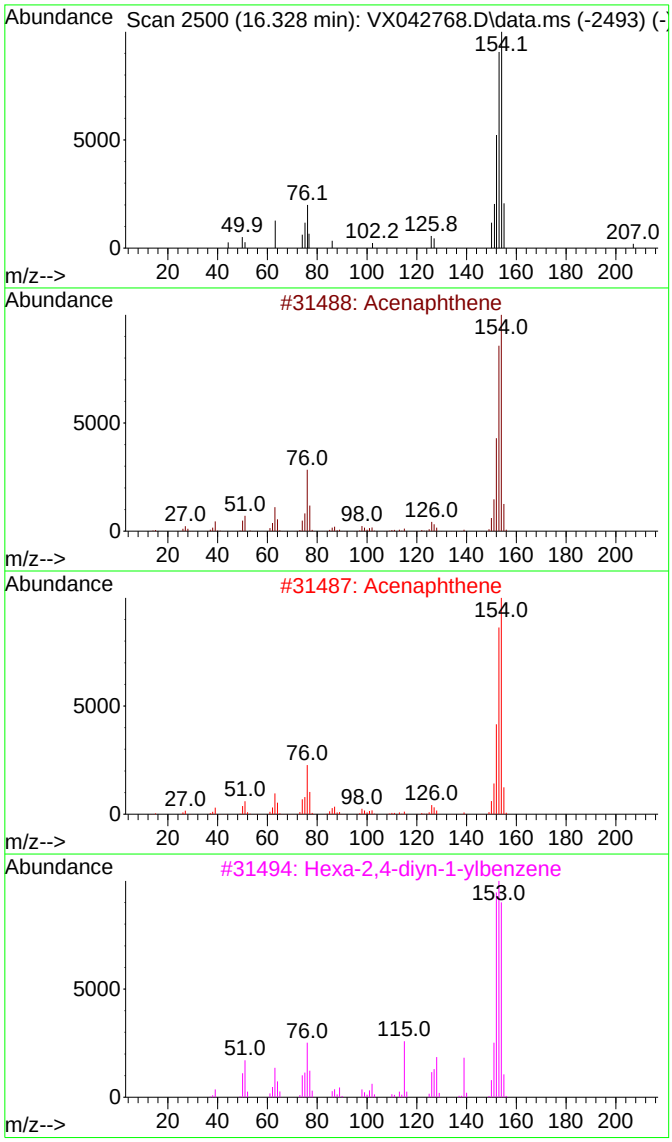
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM072624WMA.M
Quant Title : VOC Analysis

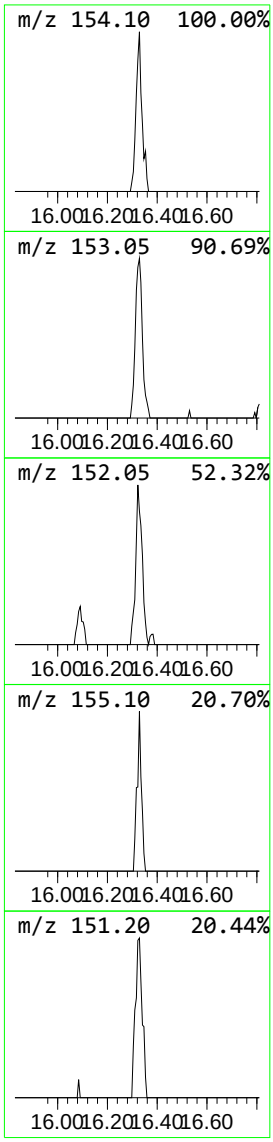
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Hexa-2,4-diyn-1-ylbenzene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.328	2.63 ug/L	15829	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acenaphthene	154	C12H10	000083-32-9	58
2	Acenaphthene	154	C12H10	000083-32-9	58
3	Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	52
4	Acenaphthene	154	C12H10	000083-32-9	49
5	Acenaphthene	154	C12H10	000083-32-9	49





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
Data File : VX042768.D
Acq On : 31 Jul 2024 13:17
Operator : JC/MD
Sample : P3361-04ME
Misc : 10.82g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20N8ME

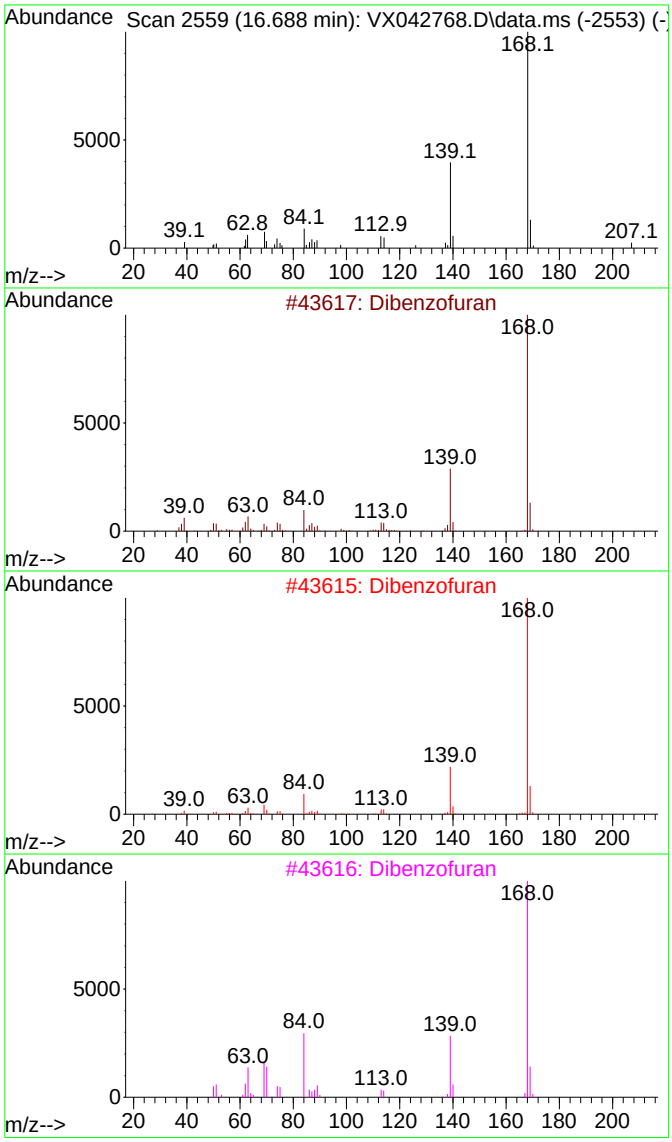
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM072624WMA.M
Quant Title : VOC Analysis

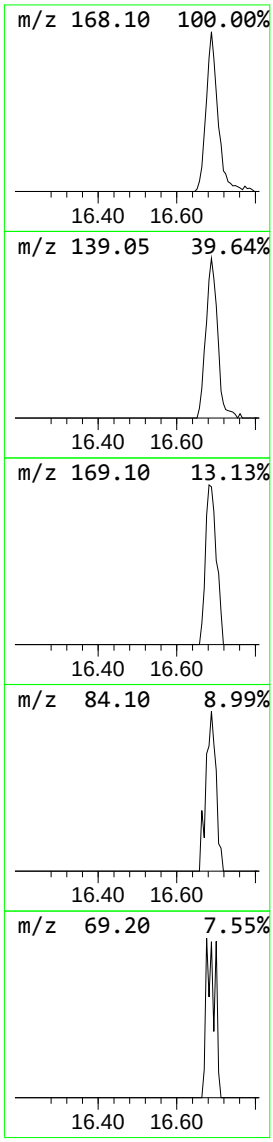
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 9H-Pyrido[3,4-b]indole Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.688	4.19 ug/L	25272	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	91
3	Dibenzofuran	168	C12H8O	000132-64-9	64
4	9H-Pyrido[3,4-b]indole	168	C11H8N2	000244-63-3	58
5	1-Naphthalenecarbonitrile, 8-amino-	168	C11H8N2	038515-13-8	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
Data File : VX042768.D
Acq On : 31 Jul 2024 13:17
Operator : JC/MD
Sample : P3361-04ME
Misc : 10.82g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20N8ME

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	5.2	ug/L	28408	1	6.757	273047	50.0
Azulene	13.774	17.0	ug/L	102301	3	12.024	301459	50.0
Benzocyclohepta...	14.640	2.5	ug/L	15164	3	12.024	301459	50.0
Hexa-2,4-diyn-1...	16.328	2.6	ug/L	15829	3	12.024	301459	50.0
9H-Pyrido[3,4-b...	16.688	4.2	ug/L	25272	3	12.024	301459	50.0