LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
Data File : VX042769.D
Acq On : 31 Jul 2024 13:40
Operator : JC/MD
Sample : P3361-22ME
Misc : 10.57g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : E20Q2ME

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: VX042769.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	27	rBV	15536	17453	4.94%	1.127%
2	1.368	43	46	48	rBV2	2311	2651	0.75%	0.171%
3	2.270	189	194	201	rBV2	11084	19568	5.54%	1.263%
4	2.459	223	225	227	rBV2	307	249	0.07%	0.016%
5	2.550	236	240	242	rBB2	247	287	0.08%	0.019%
6	2.691	262	263	267	rBB	201	202	0.06%	0.013%
7	2.776	273	277	287	rVB3	1314	3003	0.85%	0.194%
8	2.947	296	305	315	rBB2	3415	9304	2.64%	0.601%
9	3.130	329	335	338	rBB	174	274	0.08%	0.018%
10	3.245	349	354	355	rBB	187	223	0.06%	0.014%
11	3.294	360	362	365	rBB	169	176	0.05%	0.011%
12	3.550	402	404	407	rBB	168	173	0.05%	0.011%
13	4.349	533	535	540	rBB2	180	267	0.08%	0.017%
14	4.501	554	560	565	rBV3	3440	8980	2.54%	0.580%
15	4.684	585	590	594	rBV2	556	1271	0.36%	0.082%
16	4.898	623	625	627	rBV	215	217	0.06%	0.014%
17	5.056	641	651	666	rBB2	11300	34270	9.71%	2.212%
18	5.373	699	703	704	rBV	181	226	0.06%	0.015%
19	5.416	707	710	713	rBV2	286	327	0.09%	0.021%
20	5.544	729	731	733	rVV	258	228	0.06%	0.015%
21	5.574	733	736	738	rVB	206	209	0.06%	0.013%
22	5.836	775	779	782	rBB2	199	242	0.07%	0.016%
23	5.958	791	799	813	rBV3	31118	85534	24.23%	5.521%
24	6.117	824	825	828	rVV	192	180	0.05%	0.012%
25	6.178	834	835	839	rBV	146	192	0.05%	0.012%
26	6.373	861	867	872	rBV4	1166	2162	0.61%	0.140%
27	6.629	906	909	912	rBB	126	201	0.06%	0.013%
28	6.672	913	916	919	rBB2	127	164	0.05%	0.011%
29	6.757	920	930	944	rBV2	117643	289422	81.99%	18.681%
30	7.141	987	993	999	rBV5	1486	3350	0.95%	0.216%
31	7.306	1013	1020	1029	rBV2	16197	36420	10.32%	2.351%
32	7.373	1029	1031	1033	rVB2	511	322	0.09%	0.021%
33	7.434	1037	1041	1044	rBB	149	212	0.06%	0.014%
34	7.726	1087	1089	1092	rBB	203	193	0.05%	0.012%
35	7.970	1127	1129	1131	rBV	463	403	0.11%	0.026%
36	8.147	1156	1158	1161	rBV	188	206	0.06%	0.013%

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Misc : 10.57g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20Q2ME

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	8.257	1174	1176	1179	rVV	407	391	0.11%	0.025%
38	8.330	1183	1188	1197	rBV	8887	15426	4.37%	0.996%
39	8.647	1234	1240	1250	rBV	43995	73531	20.83%	4.746%
40	8.958	1286	1291	1302	rVB2	5612	10122	2.87%	0.653%
41	9.074	1308	1310	1313	rBV	171	181	0.05%	0.012%
42	9.116	1315	1317	1320	rBB	251	234	0.07%	0.015%
43	9.275	1341	1343	1347	rBV	576	601	0.17%	0.039%
44	9.397	1358	1363	1373	rBV2	13864	32720	9.27%	2.112%
45	9.659	1404	1406	1408	rBV	204	238	0.07%	0.015%
46	9.714	1412	1415	1421	rVB3	1043	1583	0.45%	0.102%
47	9.793	1426	1428	1433	rBV3	158	295	0.08%	0.019%
48	9.927	1448	1450	1452	rBV3	202	174	0.05%	0.011%
49	10.055	1465	1471	1482	rBV	248363	352995	100.00%	22.785%
50	10.202	1493	1495	1499	rVB2	625	721	0.20%	0.047%
51	10.232	1499	1500	1503	rBV	263	281	0.08%	0.018%
52	10.305	1509	1512	1518	rVB2	314	556	0.16%	0.036%
53	10.488	1540	1542	1546	rBB	239	305	0.09%	0.020%
54	10.543	1547	1551	1554	rBB	185	204	0.06%	0.013%
55	10.647	1565	1568	1571	rBB	356	416	0.12%	0.027%
56	10.854	1601	1602	1605	rBV	194	166	0.05%	0.011%
57	10.915	1607	1612	1614	rBV	224	274	0.08%	0.018%
58	10.964	1618	1620	1626	rBV	226	417	0.12%	0.027%
59	11.195	1651	1658	1667	rBV	32913	45195	12.80%	2.917%
60	11.463	1699	1702	1706	rBV	298	444	0.13%	0.029%
61	11.579	1718	1721	1723	rBV	162	196	0.06%	0.013%
62	11.646	1728	1732	1734	rBV	277	244	0.07%	0.016%
63	11.689	1736	1739	1740	rBV	192	155	0.04%	0.010%
64	11.750	1746	1749	1755	rBB	363	580	0.16%	0.037%
65	11.927	1774	1778	1780	rBB	221	235	0.07%	0.015%
66	11.969	1781	1785	1788	rBV2	350	488	0.14%	0.031%
67	12.024	1788	1794	1802	rBV	251211	323023	91.51%	20.850%
68	12.244	1826	1830	1834	rBV2	1172	1755	0.50%	0.113%
69	12.317	1837	1842	1855	rBV	48265	66566	18.86%	4.297%
70	12.579	1882	1885	1887	rBB	289	278	0.08%	0.018%
71	12.664	1895	1899	1904	rBB2	212	401	0.11%	0.026%
72	12.768	1908	1916	1917	rBV2	1967	3323	0.94%	0.214%
73	13.085	1967	1968	1971	rVB	444	383	0.11%	0.025%
74	13.128	1973	1975	1979	rVB	650	458	0.13%	0.030%
75	13.213	1986	1989	1991	rVB	208	257	0.07%	0.017%
76	13.250	1993	1995	1997	rBV	355	357	0.10%	0.023%

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Sample : P3361-22ME
Misc : 10.57g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : E20Q2ME

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	13.359	2011	2013	2015	rBV	187	166	0.05%	0.011%
78	13.433	2022	2025	2027	rBV	244	248	0.07%	0.016%
79	13.573	2047	2048	2052	rBB	205	172	0.05%	0.011%
80	13.640	2057	2059	2062	rBV	397	533	0.15%	0.034%
81	13.713	2070	2071	2074	rBV	372	309	0.09%	0.020%
82	13.774	2076	2081	2090	rBV	39058	55888	15.83%	3.607%
83	13.939	2106	2108	2111	rBV	216	205	0.06%	0.013%
84	14.042	2121	2125	2128	rBV2	582	780	0.22%	0.050%
85	14.128	2135	2139	2146	rBV3	2362	3646	1.03%	0.235%
86	14.274	2159	2163	2164	rBB3	249	279	0.08%	0.018%
87	14.439	2188	2190	2192	rVB2	177	155	0.04%	0.010%
88	14.463	2192	2194	2197	rBB2	171	217	0.06%	0.014%
89	14.560	2209	2210	2213	rVB	384	246	0.07%	0.016%
90	14.609	2214	2218	2220	rBV2	512	618	0.18%	0.040%
91	14.640	2220	2223	2228	rVV	5657	7286	2.06%	0.470%
92	14.719	2232	2236	2237	rVV	232	273	0.08%	0.018%
93	14.749	2239	2241	2243	rVV2	612	683	0.19%	0.044%
94	14.780	2243	2246	2253	rVB2	2943	4184	1.19%	0.270%
95	15.213	2312	2317	2323	rBV3	1672	2566	0.73%	0.166%
96	15.341	2334	2338	2343	rBV4	591	1391	0.39%	0.090%
97	15.481	2358	2361	2364	rBV3	819	1033	0.29%	0.067%
98	15.652	2388	2389	2392	rBV2	729	523	0.15%	0.034%
99	16.091	2458	2461	2462	rBV	483	387	0.11%	0.025%
100	16.688	2553	2559	2567	rBV2	6312	12538	3.55%	0.809%

Sum of corrected areas: 1549256

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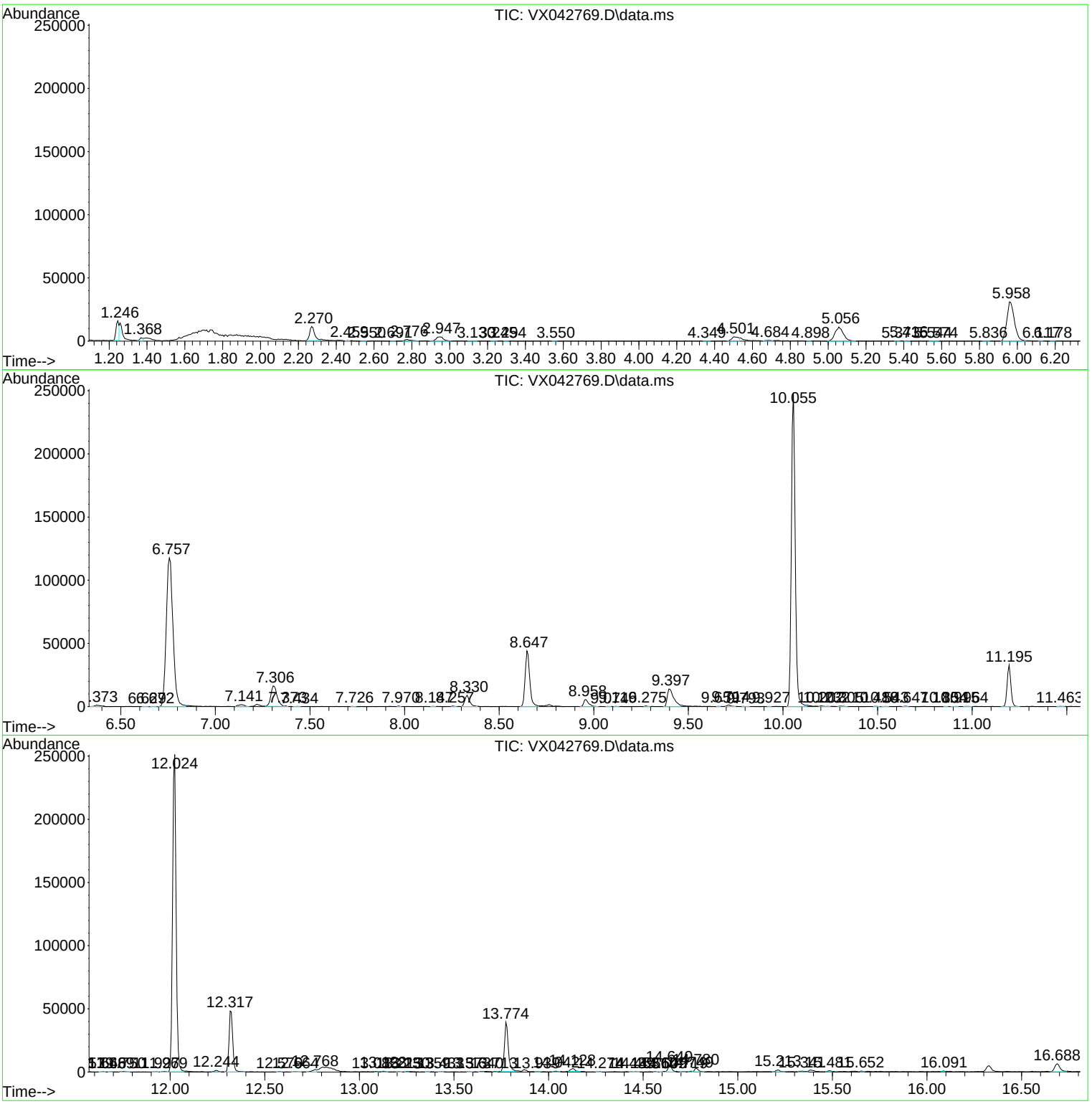
Misc : 10.57g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20Q2ME

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



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Instrument :
MSVOA_X
ClientSampleId :
E20Q2ME

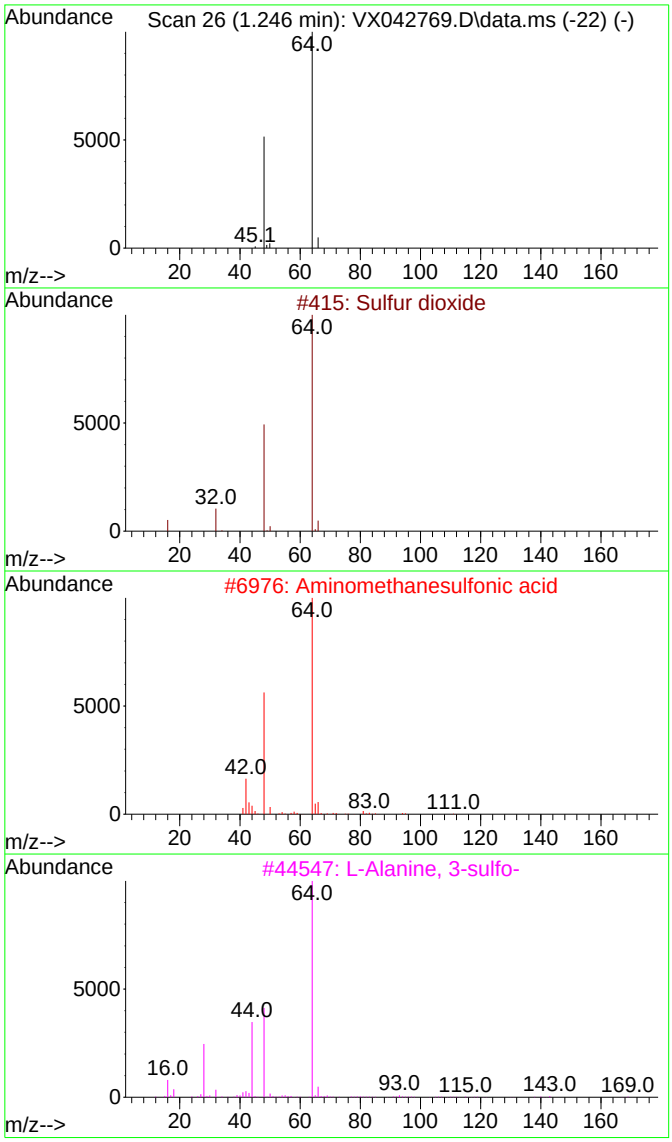
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM072624WMA.M
Quant Title : VOC Analysis

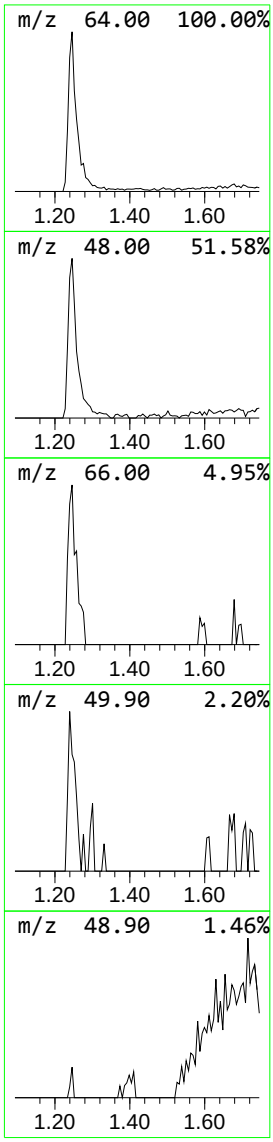
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	3.02 ug/L	17453	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	74
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9





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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20Q2ME

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

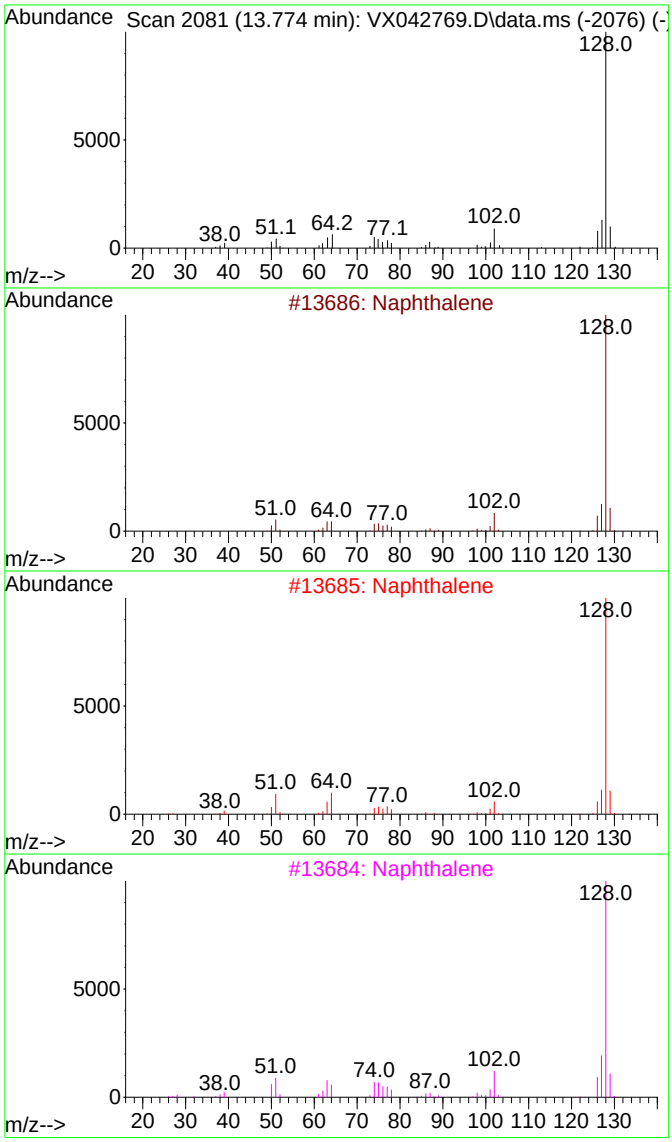
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

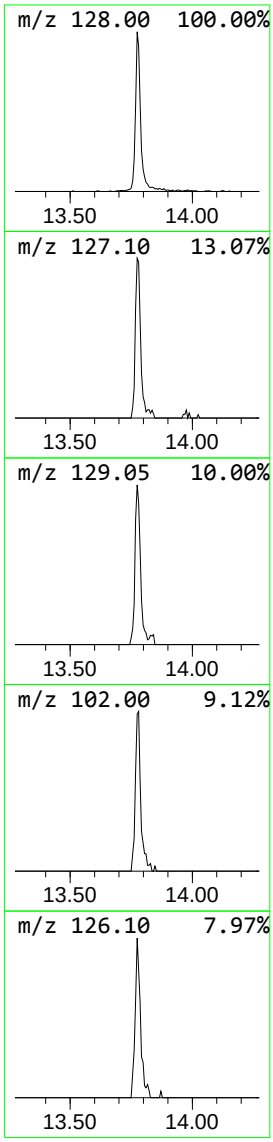
****

Peak Number 3 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	8.65 ug/L	55888	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene	128	C10H8	000091-20-3	94
2	Naphthalene	128	C10H8	000091-20-3	91
3	Naphthalene	128	C10H8	000091-20-3	91
4	Naphthalene	128	C10H8	000091-20-3	91
5	Azulene	128	C10H8	000275-51-4	91





Tentatively Identified Compound (LSC) summary

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Instrument :
MSVOA_X
ClientSampleId :
E20Q2ME

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	3.0	ug/L	17453	1	6.763	289422	50.0
Azulene	13.774	8.7	ug/L	55888	3	12.024	323023	50.0