LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU013025\
Data File : VU063106.D
Acq On : 30 Jan 2025 18:24
Operator : MD/SY
Sample : Q1148-05
Misc : 10.00g/10.0mL/100uL5.0mL/MSVOA_U/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
XA174

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\SFAMULM013025WMA.M
Title : VOC Analysis

Signal : TIC: VU063106.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.351	15	19	22	rBV3	1038	1001	0.03%	0.004%
2	1.474	47	57	66	rBV2	5304	11619	0.40%	0.042%
3	1.592	84	94	116	rVB	53258	84431	2.88%	0.307%
4	1.866	174	179	195	rVB	21607	28664	0.98%	0.104%
5	2.284	305	309	315	rBV	171	171	0.01%	0.001%
6	2.345	324	328	333	rVB2	274	204	0.01%	0.001%
7	2.428	350	354	359	rBV	246	223	0.01%	0.001%
8	2.531	374	386	404	rBV	104339	169029	5.76%	0.615%
9	2.625	404	415	448	rBV	131341	252527	8.60%	0.918%
10	2.760	453	457	469	rVB	1657	2199	0.07%	0.008%
11	2.943	505	514	525	rBV	10154	19272	0.66%	0.070%
12	3.020	525	538	573	rVV	192299	387817	13.21%	1.410%
13	3.165	573	583	600	rVB2	3706	8985	0.31%	0.033%
14	3.351	621	641	669	rBV	520370	1367304	46.58%	4.972%
15	3.554	701	704	706	rBV2	266	185	0.01%	0.001%
16	3.670	729	740	753	rBV5	4275	9417	0.32%	0.034%
17	3.908	810	814	817	rBV2	187	194	0.01%	0.001%
18	4.136	878	885	888	rBV2	203	271	0.01%	0.001%
19	4.322	937	943	944	rBV2	146	136	0.00%	0.000%
20	4.338	944	948	950	rVV2	193	189	0.01%	0.001%
21	4.370	954	958	962	rVB2	247	206	0.01%	0.001%
22	4.435	975	978	982	rBV	176	184	0.01%	0.001%
23	4.644	1025	1043	1056	rBV2	245609	644880	21.97%	2.345%
24	4.952	1135	1139	1140	rBV	761	552	0.02%	0.002%
25	5.046	1153	1168	1197	rVB	92481	209404	7.13%	0.762%
26	5.149	1197	1200	1204	rBV2	234	206	0.01%	0.001%
27	5.245	1222	1230	1231	rBV2	219	272	0.01%	0.001%
28	5.274	1237	1239	1242	rBV2	219	152	0.01%	0.001%
29	5.406	1276	1280	1281	rBV	420	301	0.01%	0.001%
30	5.419	1281	1284	1290	rVV3	827	1051	0.04%	0.004%
31	5.506	1294	1311	1342	rVB	325430	719050	24.49%	2.615%
32	5.705	1355	1373	1379	rBV2	193462	464901	15.84%	1.691%
33	5.756	1380	1389	1423	rVB2	739921	1670888	56.92%	6.076%
34	5.991	1458	1462	1465	rBV2	183	163	0.01%	0.001%
35	6.030	1471	1474	1485	rVB3	324	531	0.02%	0.002%
36	6.123	1501	1503	1508	rVB2	161	134	0.00%	0.000%

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Misc : 10.00g/10.0mL/100uL5.0mL/MSVOA_U/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
XA174

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\SFAMULM013025WMA.M
Title : VOC Analysis

37	6.235	1526	1538	1564	rBV	160380	314949	10.73%	1.145%
38	6.361	1574	1577	1583	rVB2	260	251	0.01%	0.001%
39	6.483	1610	1615	1616	rBV2	178	153	0.01%	0.001%
40	6.528	1616	1629	1651	rBV	523563	995789	33.92%	3.621%
41	6.676	1663	1675	1705	rVB	107920	218339	7.44%	0.794%
42	6.817	1717	1719	1723	rVB2	283	200	0.01%	0.001%
43	6.904	1732	1746	1772	rBV	331159	631983	21.53%	2.298%
44	7.094	1791	1805	1826	rBV	340344	665862	22.68%	2.421%
45	7.213	1832	1842	1862	rVB2	15423	31572	1.08%	0.115%
46	7.441	1907	1913	1919	rBV3	611	887	0.03%	0.003%
47	7.554	1937	1948	1954	rVV2	65129	115634	3.94%	0.421%
48	7.595	1954	1961	1983	rVV	143117	263055	8.96%	0.957%
49	7.676	1984	1986	1990	rVB2	282	173	0.01%	0.001%
50	7.785	2006	2020	2040	rBV	432940	936101	31.89%	3.404%
51	7.885	2040	2051	2062	rVV	240099	415621	14.16%	1.511%
52	7.956	2062	2073	2097	rVB	853370	1472535	50.16%	5.355%
53	8.171	2130	2140	2163	rVB	42876	81406	2.77%	0.296%
54	8.255	2163	2166	2168	rVB2	412	209	0.01%	0.001%
55	8.271	2168	2171	2178	rVB2	174	201	0.01%	0.001%
56	8.338	2190	2192	2195	rVB	279	179	0.01%	0.001%
57	8.390	2195	2208	2231	rBV	488125	911104	31.04%	3.313%
58	8.541	2242	2255	2272	rBV	299695	499229	17.01%	1.816%
59	8.631	2272	2283	2290	rVV	158687	285644	9.73%	1.039%
60	8.679	2291	2298	2323	rVV	350482	660702	22.51%	2.403%
61	8.801	2324	2336	2358	rVB	164897	312539	10.65%	1.137%
62	8.914	2358	2371	2394	rBV	324981	575842	19.62%	2.094%
63	9.409	2513	2525	2552	rBV	249956	431382	14.69%	1.569%
64	9.560	2559	2572	2596	rBV	1073947	1712072	58.32%	6.226%
65	9.682	2598	2610	2638	rVB	672503	1109221	37.78%	4.034%
66	9.930	2684	2687	2691	rVV	233	173	0.01%	0.001%
67	10.100	2724	2740	2781	rVV3	1456660	2935682	100.00%	10.676%
68	10.283	2784	2797	2819	rVB	234787	406734	13.85%	1.479%
69	10.393	2827	2831	2833	rBV2	286	164	0.01%	0.001%
70	10.480	2851	2858	2867	rVB4	1443	2360	0.08%	0.009%
71	10.525	2867	2872	2874	rBV2	220	217	0.01%	0.001%
72	10.772	2927	2949	2957	rBV2	609739	1295251	44.12%	4.710%
73	10.814	2958	2962	2979	rVB	315713	446635	15.21%	1.624%
74	11.000	3016	3020	3022	rBV2	291	275	0.01%	0.001%
75	11.090	3040	3048	3056	rBV3	867	1569	0.05%	0.006%
76	11.213	3082	3086	3089	rBV	179	169	0.01%	0.001%

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ClientSampleId :
XA174

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM013025WMA.M
Title : VOC Analysis

77	11.418	3142	3150	3157	rBV3	3153	4370	0.15%	0.016%
78	11.470	3157	3166	3175	rVB3	1805	2701	0.09%	0.010%
79	11.737	3238	3249	3260	rBV	157019	246281	8.39%	0.896%
80	11.827	3260	3277	3304	rVB2	689675	1462120	49.81%	5.317%
81	12.200	3376	3393	3434	rBV2	777150	1583326	53.93%	5.758%
82	12.348	3437	3439	3443	rVB2	351	195	0.01%	0.001%
83	12.467	3470	3476	3481	rVB3	1646	1469	0.05%	0.005%
84	12.766	3557	3569	3574	rBV3	955	1555	0.05%	0.006%
85	12.801	3574	3580	3582	rBV3	154	193	0.01%	0.001%
86	13.142	3681	3686	3689	rBV2	235	243	0.01%	0.001%
87	13.225	3706	3712	3716	rBV3	463	525	0.02%	0.002%
88	13.602	3825	3829	3832	rBV2	215	214	0.01%	0.001%
89	13.840	3895	3903	3912	rVB3	3807	5492	0.19%	0.020%
90	14.007	3952	3955	3962	rVB3	803	817	0.03%	0.003%
91	14.078	3965	3977	4008	rBV	233048	396504	13.51%	1.442%
92	14.319	4048	4052	4054	rBV3	700	580	0.02%	0.002%
93	14.971	4252	4255	4259	rBV	325	256	0.01%	0.001%
94	14.994	4259	4262	4267	rVB3	368	338	0.01%	0.001%
95	15.023	4268	4271	4273	rBV2	293	187	0.01%	0.001%
96	15.213	4327	4330	4334	rBV3	228	264	0.01%	0.001%
97	16.077	4596	4599	4601	rBV2	353	206	0.01%	0.001%
98	16.164	4623	4626	4631	rBV3	366	433	0.01%	0.002%
99	16.360	4684	4687	4690	rBV	385	259	0.01%	0.001%
100	16.643	4771	4775	4780	rBV3	604	788	0.03%	0.003%

Sum of corrected areas: 27498092

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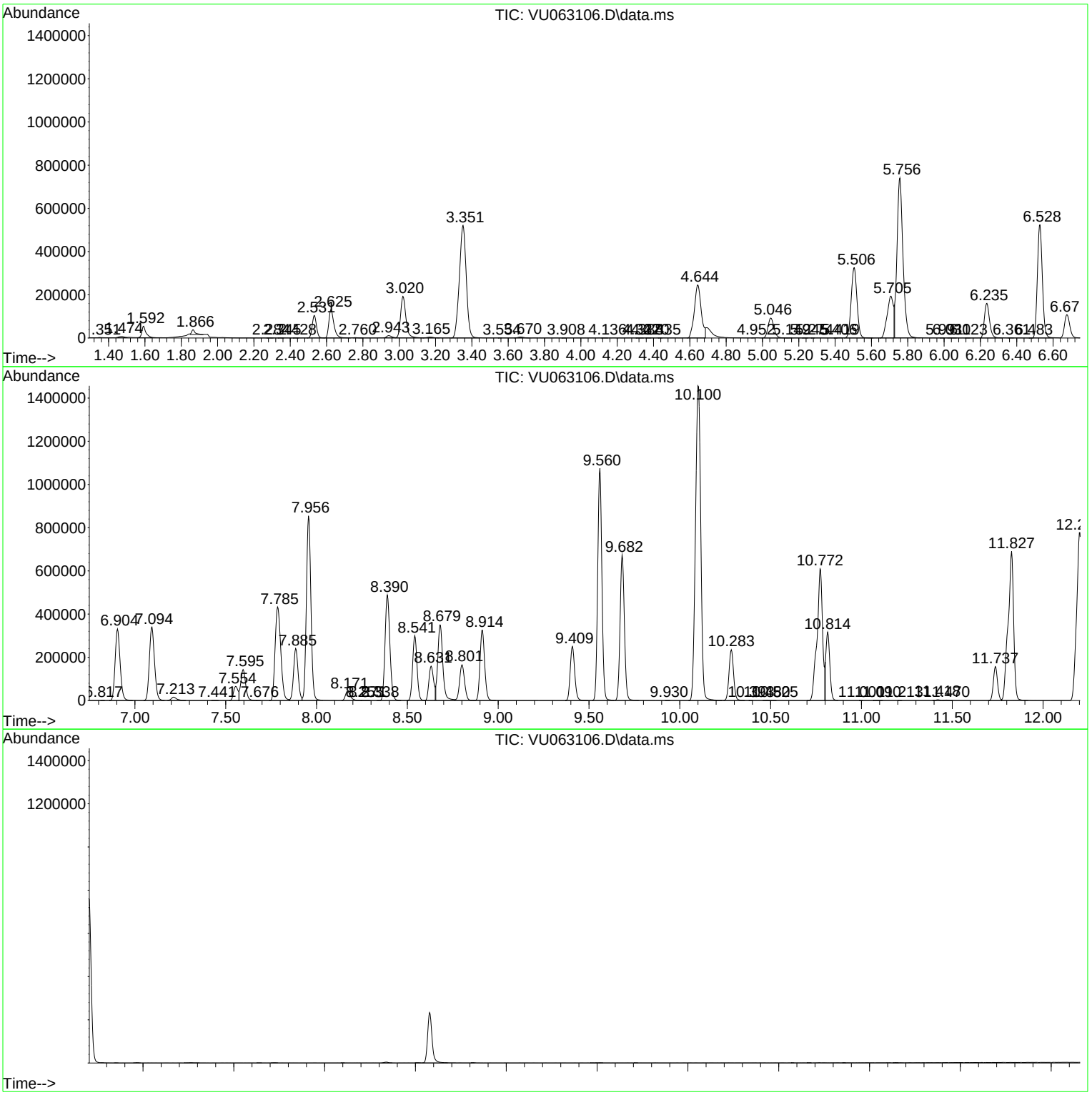
Instrument :
MSVOA_U
ClientSampleId :
XA174

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM013025WMA.M
Quant Title : VOC Analysis

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



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Instrument :
MSVOA_U
ClientSampleId :
XA174

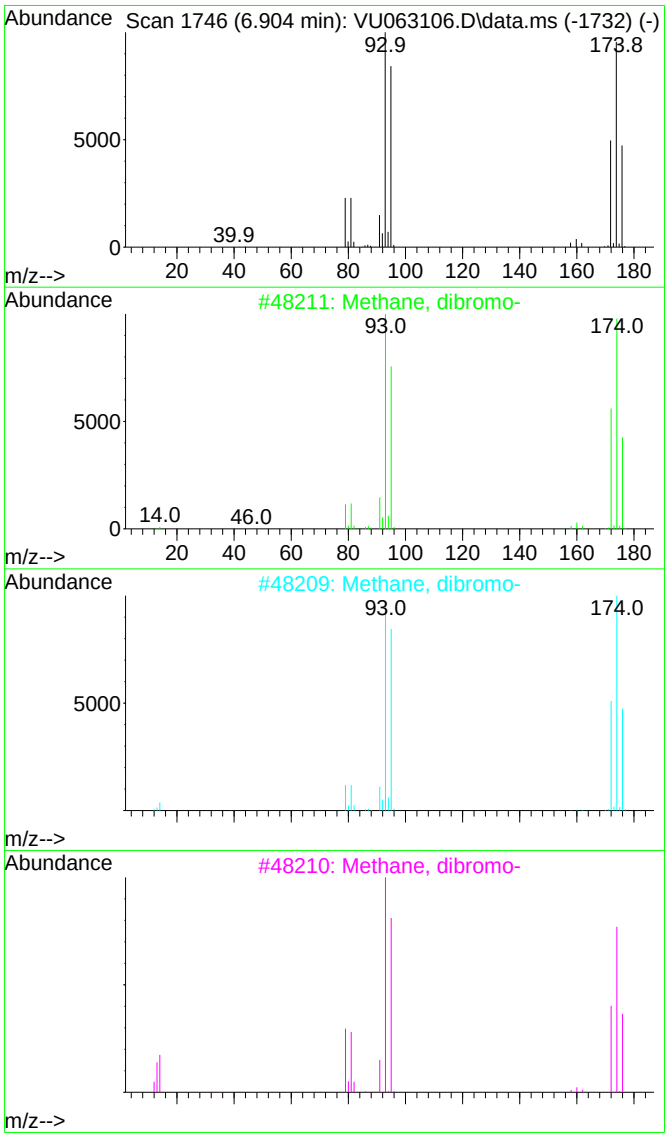
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM013025WMA.M
Quant Title : VOC Analysis

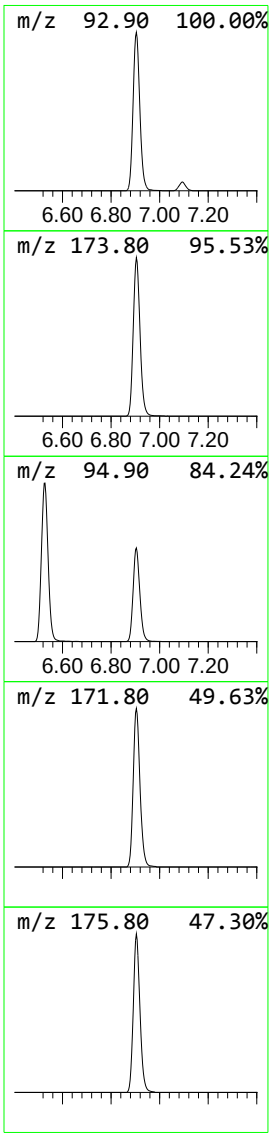
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Methane, dibromo- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.904	100.33 ug/L	631983	1,4-Difluorobenzene	6.235

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methane, dibromo-	172	CH2Br2	000074-95-3	96
2	Methane, dibromo-	172	CH2Br2	000074-95-3	96
3	Methane, dibromo-	172	CH2Br2	000074-95-3	91
4	Methane, dibromo-	172	CH2Br2	000074-95-3	90
5	Phosphorodithioic acid, O,O,S-tr...	172	C3H9O2PS2	002953-29-9	9





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Sample : Q1148-05
Misc : 10.00g/10.0mL/100uL5.0mL/MSVOA_U/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
XA174

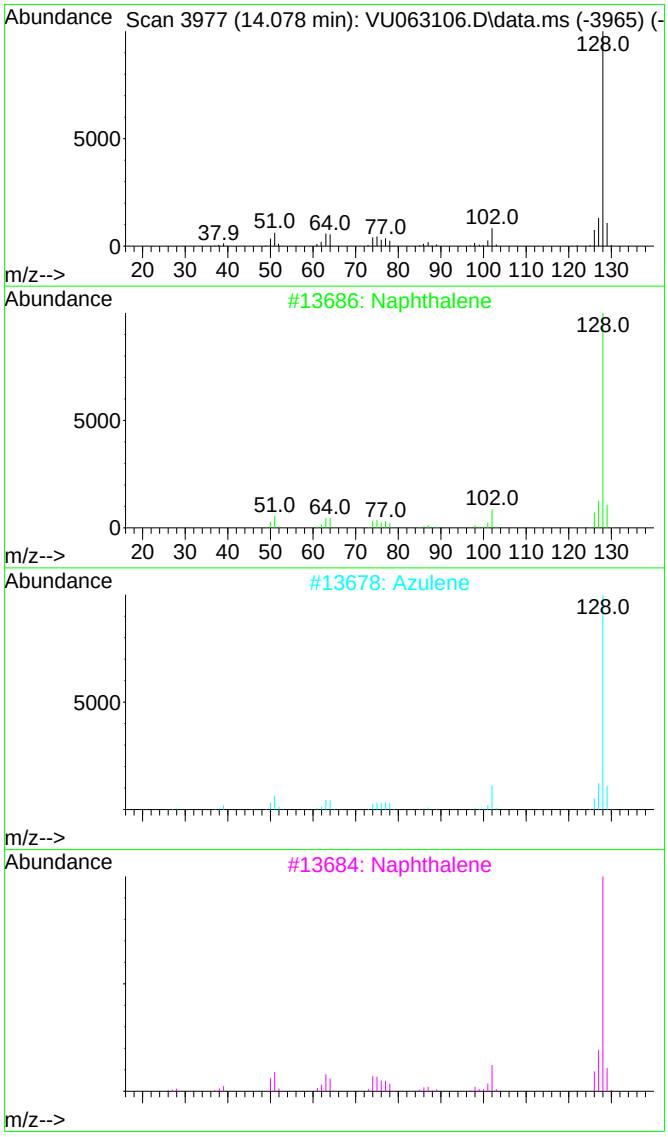
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM013025WMA.M
Quant Title : VOC Analysis

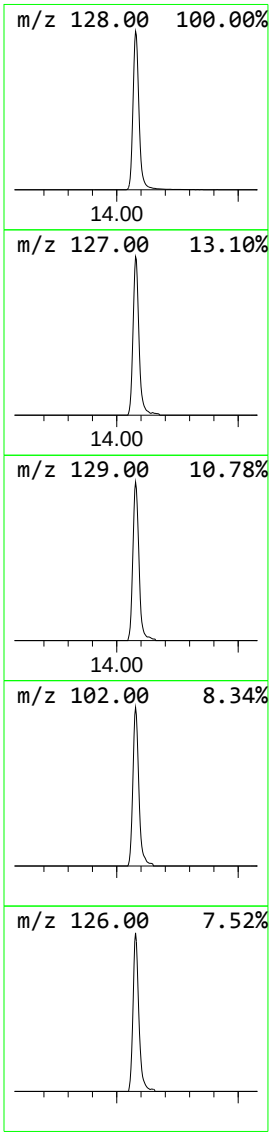
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Azulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.078	13.56 ug/L	396504	1,4-Dichlorobenzene-d4	11.804

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	Naphthalene	128	C10H8	000091-20-3	94
4	Naphthalene	128	C10H8	000091-20-3	93
5	Azulene	128	C10H8	000275-51-4	91





Tentatively Identified Compound (LSC) summary

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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
Methane, dibromo-	6.904	100.3	ug/L	631983	1	6.235	314949	50.0
Azulene	14.078	13.6	ug/L	396504	3	11.804	1462120	50.0