LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121123\
Data File : VV033203.D
Acq On : 11 Dec 2023 11:12
Operator : SY/MD
Sample : VV1211MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VBLK238

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_V\Method\SFAMVLM120123WMA.M
Title : VOC Analysis

Signal : TIC: VV033203.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.278	67	74	87	rVB	118093	123334	13.19%	1.642%
2	1.433	111	122	128	rVB9	10754	15059	1.61%	0.200%
3	1.529	144	152	165	rVB	87775	106701	11.41%	1.420%
4	1.622	178	181	186	rVB	894	719	0.08%	0.010%
5	1.651	186	190	192	rBV3	615	497	0.05%	0.007%
6	1.693	199	203	207	rVB4	696	642	0.07%	0.009%
7	1.799	233	236	242	rVB2	1180	1164	0.12%	0.015%
8	1.893	260	265	269	rVV2	695	706	0.08%	0.009%
9	2.056	305	316	341	rBV	187222	276723	29.60%	3.683%
10	2.150	341	345	347	rBV	487	455	0.05%	0.006%
11	2.368	409	413	416	rBV2	682	567	0.06%	0.008%
12	2.388	416	419	422	rBV3	860	776	0.08%	0.010%
13	2.474	442	446	448	rBV2	568	486	0.05%	0.006%
14	2.581	476	479	482	rVB	888	554	0.06%	0.007%
15	3.368	721	724	728	rVB	674	462	0.05%	0.006%
16	3.513	766	769	771	rVB	794	472	0.05%	0.006%
17	3.532	771	775	776	rBV	699	475	0.05%	0.006%
18	3.584	786	791	794	rBV2	981	809	0.09%	0.011%
19	3.642	805	809	812	rBV	925	726	0.08%	0.010%
20	3.696	821	826	830	rBV2	734	895	0.10%	0.012%
21	3.780	844	852	882	rBV	52193	138064	14.77%	1.838%
22	4.060	936	939	943	rBV2	926	580	0.06%	0.008%
23	4.246	979	997	1026	rBV2	158444	403960	43.21%	5.377%
24	4.420	1048	1051	1054	rVB2	698	475	0.05%	0.006%
25	4.529	1080	1085	1087	rBV2	755	689	0.07%	0.009%
26	4.613	1108	1111	1115	rVV	724	567	0.06%	0.008%
27	4.661	1123	1126	1135	rVB3	865	921	0.10%	0.012%
28	4.719	1139	1144	1147	rBV2	565	574	0.06%	0.008%
29	4.789	1162	1166	1170	rVB2	750	533	0.06%	0.007%
30	4.815	1170	1174	1178	rVB2	580	483	0.05%	0.006%
31	4.870	1185	1191	1194	rBV2	465	541	0.06%	0.007%
32	4.953	1200	1217	1243	rBV2	347964	934904	100.00%	12.444%
33	5.532	1384	1397	1432	rBV	301163	622612	66.60%	8.288%
34	5.828	1478	1489	1510	rVB5	14440	33480	3.58%	0.446%
35	5.986	1525	1538	1565	rBV	195094	404664	43.28%	5.386%
36	6.384	1659	1662	1666	rBV2	548	458	0.05%	0.006%

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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

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Title : VOC Analysis

37	6.487	1689	1694	1698	rBV	724	679	0.07%	0.009%
38	6.760	1775	1779	1782	rBV	525	539	0.06%	0.007%
39	6.796	1786	1790	1793	rBV	712	538	0.06%	0.007%
40	6.834	1799	1802	1804	rBV	809	542	0.06%	0.007%
41	6.912	1816	1826	1849	rBV	115408	214004	22.89%	2.849%
42	7.243	1916	1929	1955	rBV	437416	766375	81.97%	10.201%
43	7.551	2016	2025	2046	rBV	86060	153055	16.37%	2.037%
44	7.744	2082	2085	2087	rBV	678	499	0.05%	0.007%
45	7.857	2117	2120	2124	rBV2	852	785	0.08%	0.010%
46	8.024	2160	2172	2202	rBV	191618	374456	40.05%	4.984%
47	8.320	2261	2264	2267	rVB2	1012	695	0.07%	0.009%
48	8.394	2283	2287	2294	rVB3	843	1215	0.13%	0.016%
49	8.439	2295	2301	2305	rBV2	902	1172	0.13%	0.016%
50	8.532	2326	2330	2332	rBV	630	490	0.05%	0.007%
51	8.593	2345	2349	2359	rVB	1072	1341	0.14%	0.018%
52	8.654	2364	2368	2370	rBV	544	457	0.05%	0.006%
53	8.783	2397	2408	2434	rBV	470890	768153	82.16%	10.225%
54	9.124	2511	2514	2519	rVB2	1057	989	0.11%	0.013%
55	9.146	2519	2521	2527	rBV2	543	565	0.06%	0.008%
56	9.178	2527	2531	2534	rBV	592	488	0.05%	0.006%
57	9.304	2567	2570	2573	rVB	758	479	0.05%	0.006%
58	9.490	2624	2628	2629	rBV2	806	532	0.06%	0.007%
59	9.670	2681	2684	2689	rBV	597	654	0.07%	0.009%
60	9.879	2742	2749	2753	rBV	997	1531	0.16%	0.020%
61	10.153	2819	2834	2856	rBV	278210	446798	47.79%	5.947%
62	10.281	2869	2874	2877	rVB	826	682	0.07%	0.009%
63	10.320	2882	2886	2888	rBV2	920	842	0.09%	0.011%
64	10.403	2906	2912	2913	rBV	638	547	0.06%	0.007%
65	10.436	2919	2922	2926	rVB	727	519	0.06%	0.007%
66	10.484	2933	2937	2942	rBV3	888	641	0.07%	0.009%
67	10.680	2994	2998	3003	rBV2	908	901	0.10%	0.012%
68	10.854	3048	3052	3055	rBV3	991	901	0.10%	0.012%
69	11.133	3133	3139	3142	rBV5	1869	2174	0.23%	0.029%
70	11.185	3145	3155	3179	rVV	499510	779731	83.40%	10.379%
71	11.333	3197	3201	3203	rBV	812	637	0.07%	0.008%
72	11.371	3210	3213	3220	rVB3	825	887	0.09%	0.012%
73	11.429	3227	3231	3233	rBV	1059	758	0.08%	0.010%
74	11.561	3261	3272	3293	rBV	508930	805333	86.14%	10.720%
75	11.931	3382	3387	3389	rBV2	949	935	0.10%	0.012%
76	11.972	3397	3400	3406	rBV	613	579	0.06%	0.008%

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Instrument :
MSVOA_V
ClientSampleId :
VBLK238

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
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Stop Thrs : 0 Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Title : VOC Analysis

77	12.014	3410	3413	3417	rBV2	588	474	0.05%	0.006%
78	12.114	3441	3444	3447	rVB	1133	646	0.07%	0.009%
79	12.590	3585	3592	3603	rBV6	3844	6353	0.68%	0.085%
80	12.689	3620	3623	3627	rVB	894	652	0.07%	0.009%
81	12.767	3643	3647	3651	rVB	926	776	0.08%	0.010%
82	12.792	3651	3655	3658	rBV2	715	649	0.07%	0.009%
83	12.915	3690	3693	3699	rVB	1348	1116	0.12%	0.015%
84	12.953	3700	3705	3708	rBV2	1254	1344	0.14%	0.018%
85	13.201	3775	3782	3792	rBV3	8103	12787	1.37%	0.170%
86	13.297	3809	3812	3815	rBV	835	546	0.06%	0.007%
87	13.365	3828	3833	3835	rBV2	585	490	0.05%	0.007%
88	13.445	3848	3858	3869	rBV	30781	50154	5.36%	0.668%
89	13.567	3893	3896	3901	rBV3	999	872	0.09%	0.012%
90	13.593	3901	3904	3908	rBV2	539	600	0.06%	0.008%
91	13.686	3924	3933	3947	rBV3	11009	17511	1.87%	0.233%
92	13.786	3958	3964	3967	rBV2	891	1075	0.11%	0.014%
93	13.805	3967	3970	3971	rBV2	819	491	0.05%	0.007%
94	13.850	3980	3984	3990	rBV2	1005	925	0.10%	0.012%
95	13.882	3990	3994	4002	rVV	703	820	0.09%	0.011%
96	13.950	4012	4015	4021	rBV3	1213	1497	0.16%	0.020%
97	14.050	4043	4046	4048	rVV	801	467	0.05%	0.006%
98	14.898	4307	4310	4317	rBV5	1512	1799	0.19%	0.024%
99	15.117	4374	4378	4382	rBV4	803	845	0.09%	0.011%
100	15.423	4470	4473	4477	rBV2	919	897	0.10%	0.012%

Sum of corrected areas: 7512611

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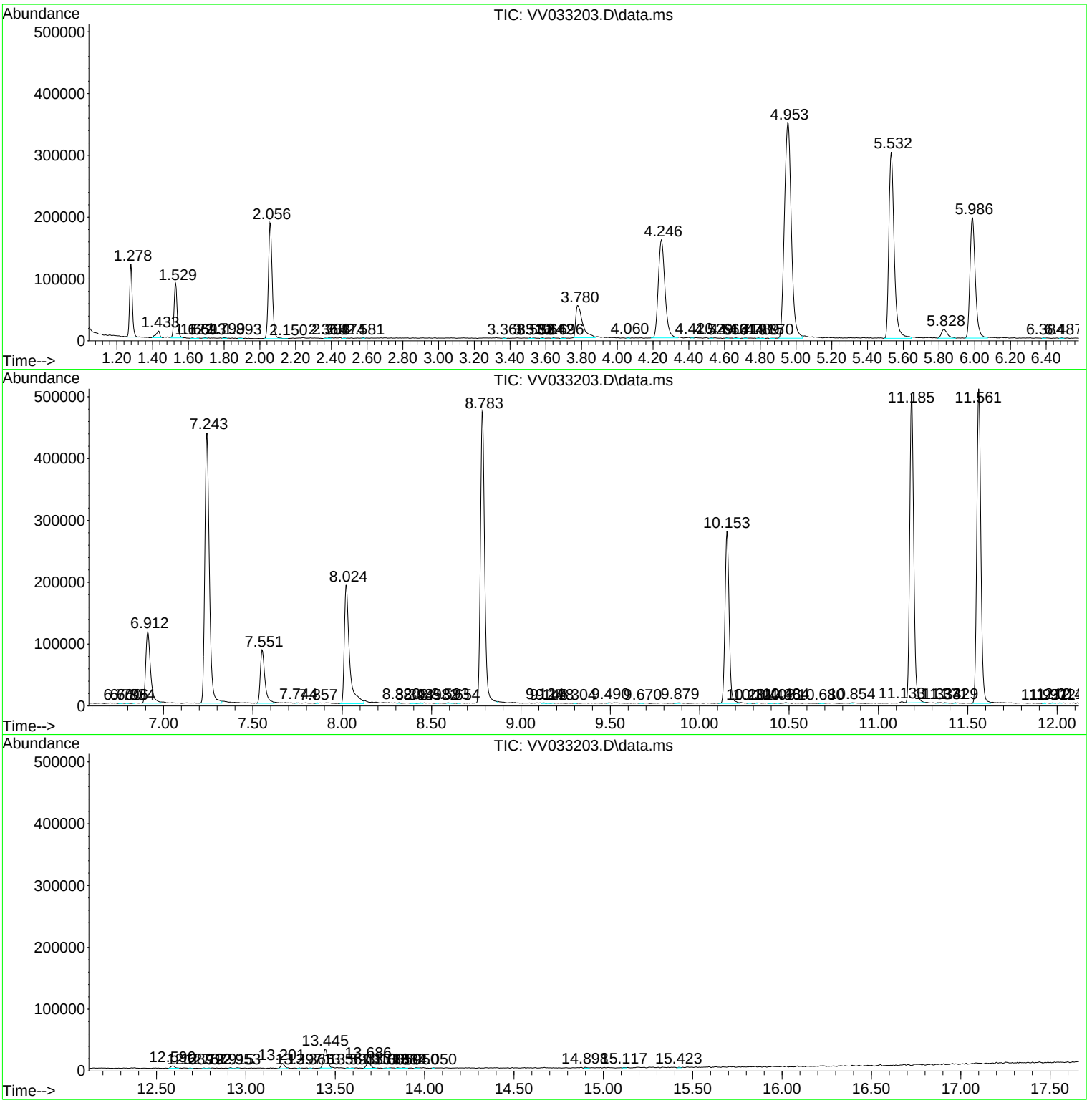
Instrument :
MSVOA_V
ClientSampleId :
VBLK238

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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



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Instrument :
MSVOA_V
ClientSampleId :
VBLK238

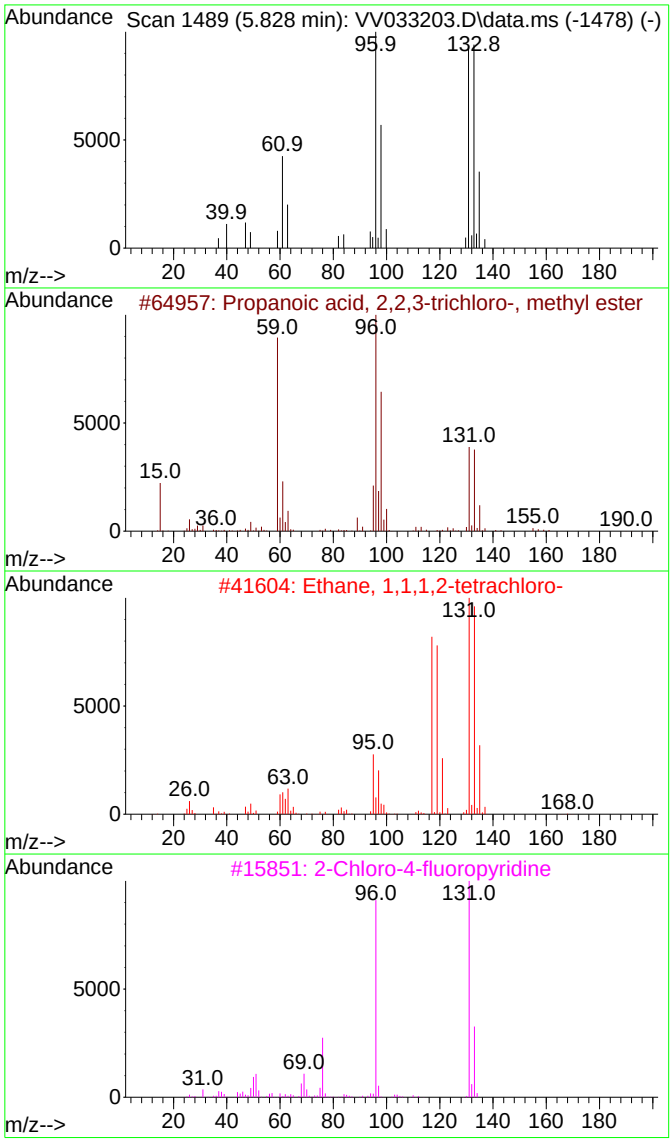
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

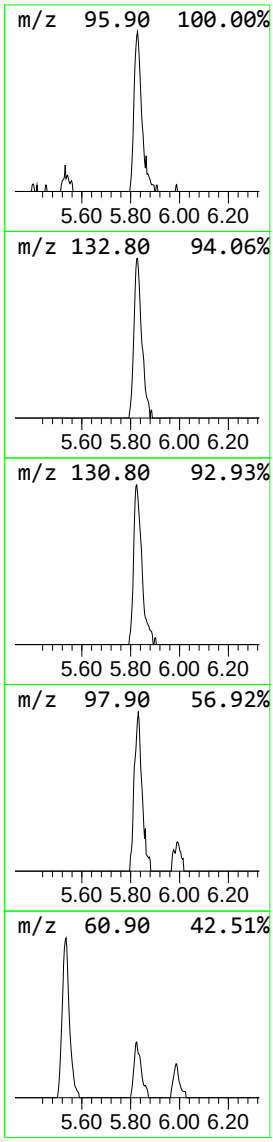
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Propanoic acid, 2,2,3-trich... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.828	2.69 ug/L	33480	1,4-Difluorobenzene	5.532

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	50
2	Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	38
3	2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	38
4	Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	35
5	2-Chloro-5-methylthiazole	133	C4H4ClNS	033342-65-3	25





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Quant Title : VOC Analysis

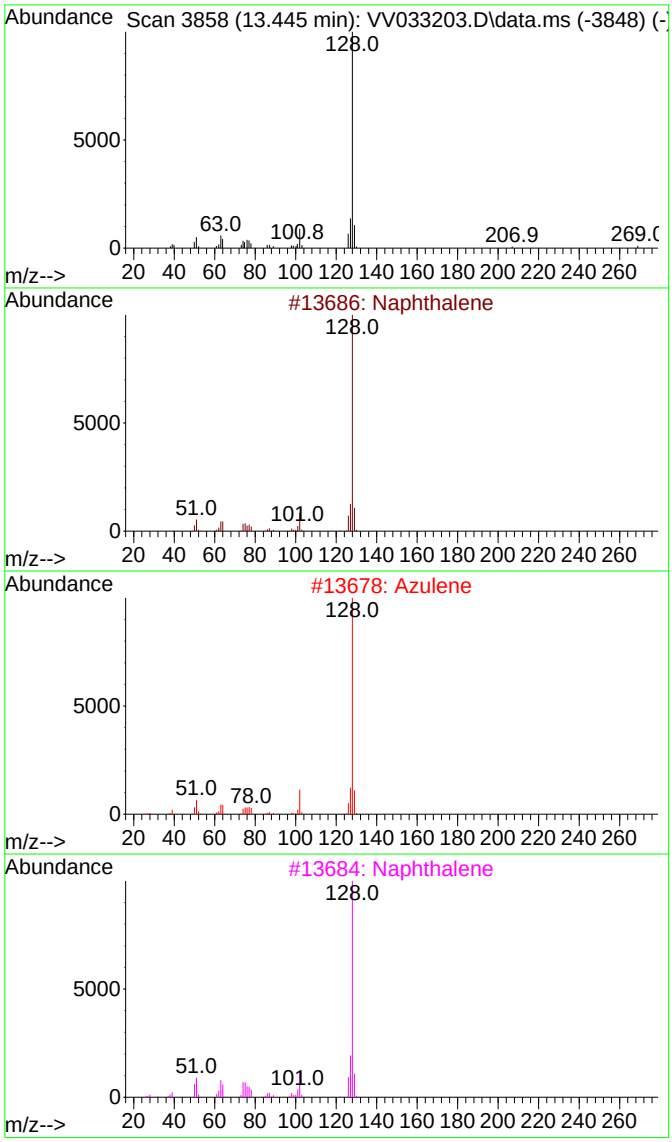
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

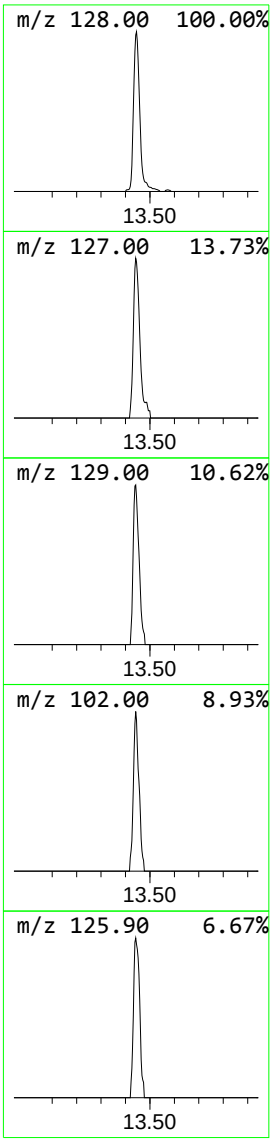
****

Peak Number 3 Azulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.445	3.22 ug/L	50154	1,4-Dichlorobenzene-d4	11.185

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene	128	C10H8	000091-20-3	95
2	Azulene	128	C10H8	000275-51-4	95
3	Naphthalene	128	C10H8	000091-20-3	91
4	Azulene	128	C10H8	000275-51-4	91
5	Naphthalene	128	C10H8	000091-20-3	90





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
Propanoic acid,...	5.828	2.7	ug/L	33480	1	5.532	622612	50.0
Azulene	13.445	3.2	ug/L	50154	3	11.185	779731	50.0