LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121721\
Data File : VU046481.D
Acq On : 17 Dec 2021 18:42
Operator : SY/MD
Sample : M5153-08 10X
Misc : 6.34g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BGL73

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\SFAMULM112921WMA.M
Title : VOC Analysis

Signal : TIC: VU046481.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.600	74	81	104	rVB	49473	64249	8.33%	1.233%
2	1.919	171	180	191	rBV	35829	50474	6.54%	0.969%
3	2.253	281	284	291	rBV2	165	197	0.03%	0.004%
4	2.571	371	383	403	rBV	93812	156222	20.25%	2.999%
5	2.703	422	424	426	rBV	126	92	0.01%	0.002%
6	2.742	431	436	441	rBB	150	221	0.03%	0.004%
7	2.806	452	456	459	rBB	141	146	0.02%	0.003%
8	2.883	476	480	483	rBB	161	150	0.02%	0.003%
9	3.047	526	531	538	rBB2	716	1054	0.14%	0.020%
10	3.083	539	542	545	rBB	137	115	0.01%	0.002%
11	3.144	557	561	564	rBB	146	124	0.02%	0.002%
12	3.189	565	575	588	rBV2	2171	4785	0.62%	0.092%
13	3.407	640	643	645	rBB	165	107	0.01%	0.002%
14	3.935	803	807	810	rBB	141	117	0.02%	0.002%
15	4.317	923	926	929	rBB	125	110	0.01%	0.002%
16	4.632	1011	1024	1047	rBV	42395	110219	14.29%	2.116%
17	4.838	1085	1088	1090	rBV	230	156	0.02%	0.003%
18	5.067	1143	1159	1176	rBV2	90866	194370	25.20%	3.731%
19	5.176	1190	1193	1195	rBV	235	130	0.02%	0.002%
20	5.276	1222	1224	1226	rBV	262	154	0.02%	0.003%
21	5.321	1234	1238	1240	rBV2	224	160	0.02%	0.003%
22	5.337	1240	1243	1248	rVB2	265	254	0.03%	0.005%
23	5.729	1344	1365	1389	rBV2	175630	474845	61.56%	9.115%
24	5.973	1439	1441	1444	rBV	134	115	0.01%	0.002%
25	6.038	1459	1461	1464	rBB	153	100	0.01%	0.002%
26	6.150	1494	1496	1499	rBB	137	97	0.01%	0.002%
27	6.185	1504	1507	1509	rBB	148	100	0.01%	0.002%
28	6.250	1513	1527	1548	rBV	169179	316668	41.05%	6.078%
29	6.353	1557	1559	1561	rVB2	234	110	0.01%	0.002%
30	6.546	1614	1619	1623	rVB2	698	702	0.09%	0.013%
31	6.693	1652	1665	1683	rBV	111980	215265	27.91%	4.132%
32	6.755	1683	1684	1687	rVB	242	100	0.01%	0.002%
33	6.822	1702	1705	1707	rBB	144	96	0.01%	0.002%
34	6.919	1732	1735	1738	rBB	184	145	0.02%	0.003%
35	7.185	1814	1818	1823	rBB2	321	363	0.05%	0.007%
36	7.279	1843	1847	1853	rBB	169	227	0.03%	0.004%

LSC Area Percent Report

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Sample : M5153-08 10X
Misc : 6.34g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGL73

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\SFAMULM112921WMA.M
Title : VOC Analysis

37	7.568	1924	1937	1953	rBV	58415	101021	13.10%	1.939%
38	7.899	2027	2040	2055	rBV	215732	364263	47.23%	6.992%
39	8.050	2084	2087	2089	rBB	134	91	0.01%	0.002%
40	8.182	2117	2128	2143	rBV	41041	68433	8.87%	1.314%
41	8.259	2146	2152	2155	rVB2	264	348	0.05%	0.007%
42	8.317	2168	2170	2172	rBV	127	94	0.01%	0.002%
43	8.468	2213	2217	2218	rBV	349	257	0.03%	0.005%
44	8.552	2238	2243	2251	rBV4	1585	2200	0.29%	0.042%
45	8.636	2256	2269	2292	rBV	140931	243031	31.51%	4.665%
46	8.851	2333	2336	2339	rBB	163	139	0.02%	0.003%
47	8.909	2350	2354	2355	rBV	592	381	0.05%	0.007%
48	9.054	2395	2399	2401	rBB	146	124	0.02%	0.002%
49	9.166	2431	2434	2436	rBV	124	107	0.01%	0.002%
50	9.224	2449	2452	2455	rBB	136	118	0.02%	0.002%
51	9.275	2465	2468	2471	rBB	178	136	0.02%	0.003%
52	9.308	2475	2478	2481	rBV	139	149	0.02%	0.003%
53	9.417	2500	2512	2536	rBV	249876	410020	53.16%	7.870%
54	9.555	2552	2555	2557	rBB	147	102	0.01%	0.002%
55	9.578	2558	2562	2564	rBV	236	153	0.02%	0.003%
56	9.639	2578	2581	2585	rBV	183	199	0.03%	0.004%
57	9.700	2598	2600	2603	rVB	297	179	0.02%	0.003%
58	9.722	2604	2607	2609	rBV	157	127	0.02%	0.002%
59	9.751	2614	2616	2619	rBV	144	131	0.02%	0.003%
60	9.806	2631	2633	2636	rBB	126	91	0.01%	0.002%
61	9.838	2641	2643	2647	rBB	125	111	0.01%	0.002%
62	9.886	2655	2658	2661	rBV	157	163	0.02%	0.003%
63	9.970	2680	2684	2689	rBB	171	227	0.03%	0.004%
64	10.002	2690	2694	2697	rBV	131	137	0.02%	0.003%
65	10.070	2712	2715	2717	rBV	124	113	0.01%	0.002%
66	10.160	2741	2743	2747	rBB	128	111	0.01%	0.002%
67	10.195	2752	2754	2756	rBV	147	97	0.01%	0.002%
68	10.288	2779	2783	2785	rBB	182	138	0.02%	0.003%
69	10.381	2810	2812	2815	rBV	127	112	0.01%	0.002%
70	10.423	2822	2825	2831	rBB	169	207	0.03%	0.004%
71	10.452	2832	2834	2838	rBV	178	173	0.02%	0.003%
72	10.500	2847	2849	2851	rBV	151	106	0.01%	0.002%
73	10.671	2897	2902	2913	rVB4	987	1072	0.14%	0.021%
74	10.758	2917	2929	2945	rBV	169220	265995	34.49%	5.106%
75	11.005	3002	3006	3007	rBV	127	114	0.01%	0.002%
76	11.060	3016	3023	3029	rBB	171	337	0.04%	0.006%

LSC Area Percent Report

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Operator : SY/MD
Sample : M5153-08 10X
Misc : 6.34g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGL73

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\SFAMULM112921WMA.M
Title : VOC Analysis

77	11.089	3029	3032	3035	rBV	184	162	0.02%	0.003%
78	11.134	3042	3046	3049	rBV	164	188	0.02%	0.004%
79	11.211	3066	3070	3072	rBV	154	149	0.02%	0.003%
80	11.256	3081	3084	3087	rBB	131	91	0.01%	0.002%
81	11.314	3095	3102	3104	rBV	158	232	0.03%	0.004%
82	11.455	3139	3146	3151	rBV2	538	754	0.10%	0.014%
83	11.536	3169	3171	3173	rBV	143	103	0.01%	0.002%
84	11.690	3216	3219	3221	rBV2	207	145	0.02%	0.003%
85	11.812	3245	3257	3274	rVB	284483	443297	57.47%	8.509%
86	12.195	3361	3376	3391	rVB	238058	375928	48.74%	7.216%
87	12.642	3512	3515	3518	rBV	188	131	0.02%	0.003%
88	12.774	3549	3556	3562	rVB2	717	958	0.12%	0.018%
89	13.024	3632	3634	3639	rBV	183	152	0.02%	0.003%
90	13.458	3766	3769	3773	rVB2	305	187	0.02%	0.004%
91	14.089	3954	3965	3979	rVB	34254	53840	6.98%	1.033%
92	14.577	4110	4117	4128	rBV	1022	1614	0.21%	0.031%
93	14.976	4238	4241	4245	rBV	188	103	0.01%	0.002%
94	15.169	4288	4301	4306	rBV4	3159	4989	0.65%	0.096%
95	15.224	4306	4318	4341	rVB	524190	771332	100.00%	14.806%
96	15.410	4364	4376	4389	rBV	224909	349982	45.37%	6.718%
97	15.954	4535	4545	4557	rVB	50038	75202	9.75%	1.443%
98	16.146	4598	4605	4613	rBV2	10267	13186	1.71%	0.253%
99	16.262	4632	4641	4658	rVB2	18892	33727	4.37%	0.647%
100	16.410	4677	4687	4693	rBV2	19380	29638	3.84%	0.569%

Sum of corrected areas: 5209736

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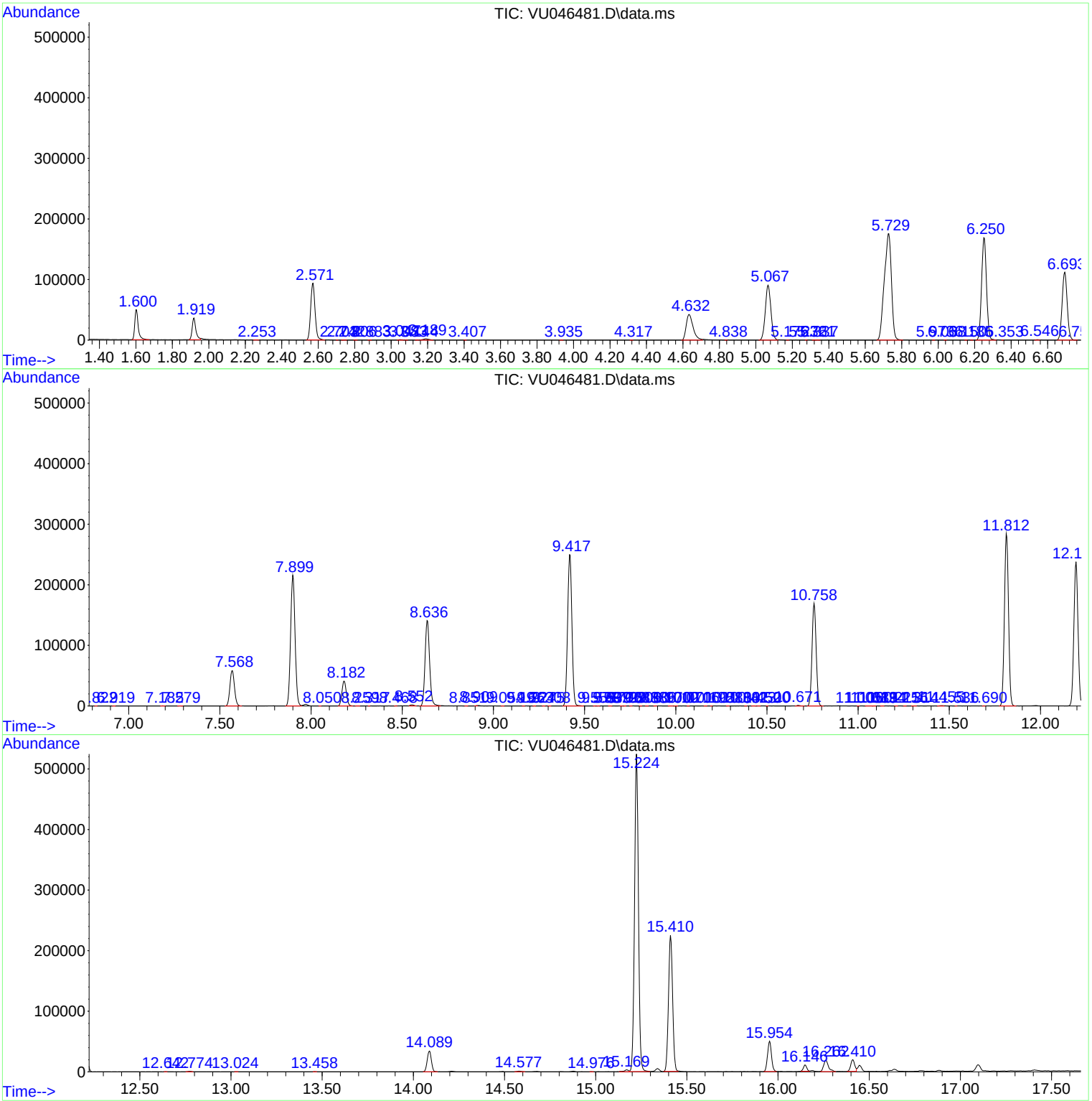
Misc : 6.34g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGL73

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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



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Instrument :
MSVOA_U
ClientSampleId :
BGL73

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

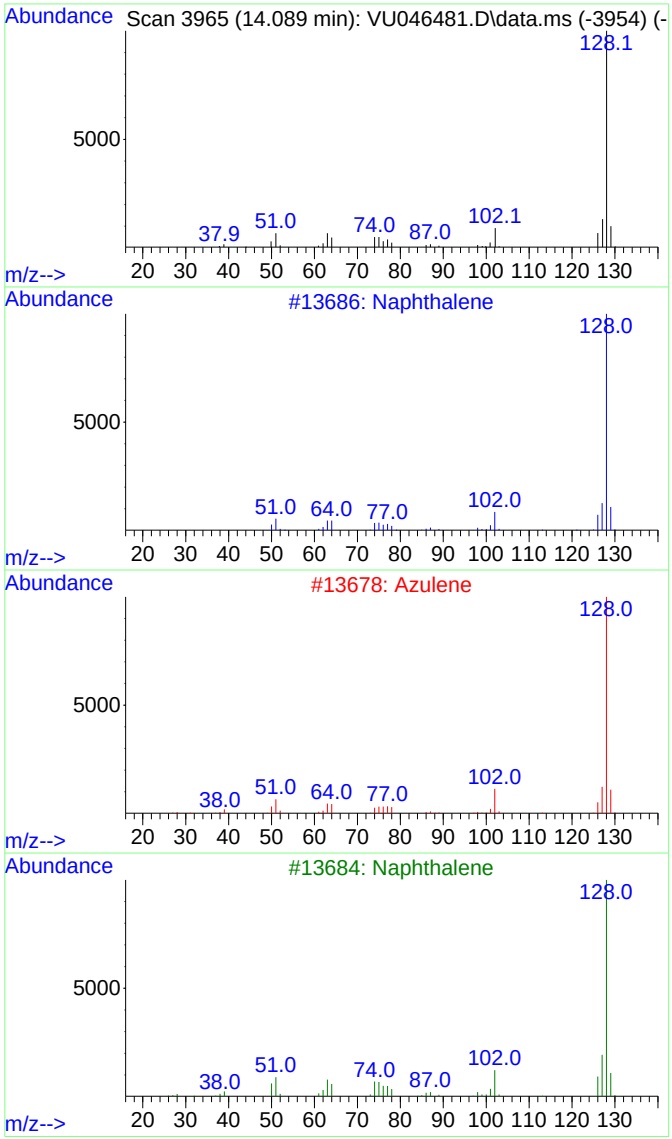
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

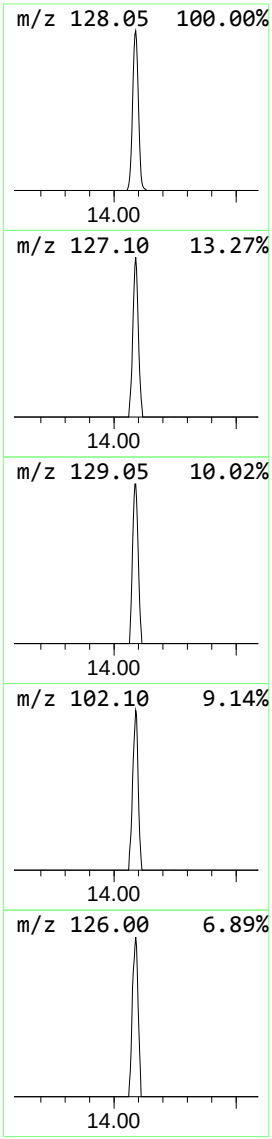
****

Peak Number 2 Azulene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.089	6.07 ug/L	53840	1,4-Dichlorobenzene-d4	11.812

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	91
4	Azulene	128	C10H8	000275-51-4	91
5	Azulene	128	C10H8	000275-51-4	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121721\
Data File : VU046481.D
Acq On : 17 Dec 2021 18:42
Operator : SY/MD
Sample : M5153-08 10X
Misc : 6.34g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGL73

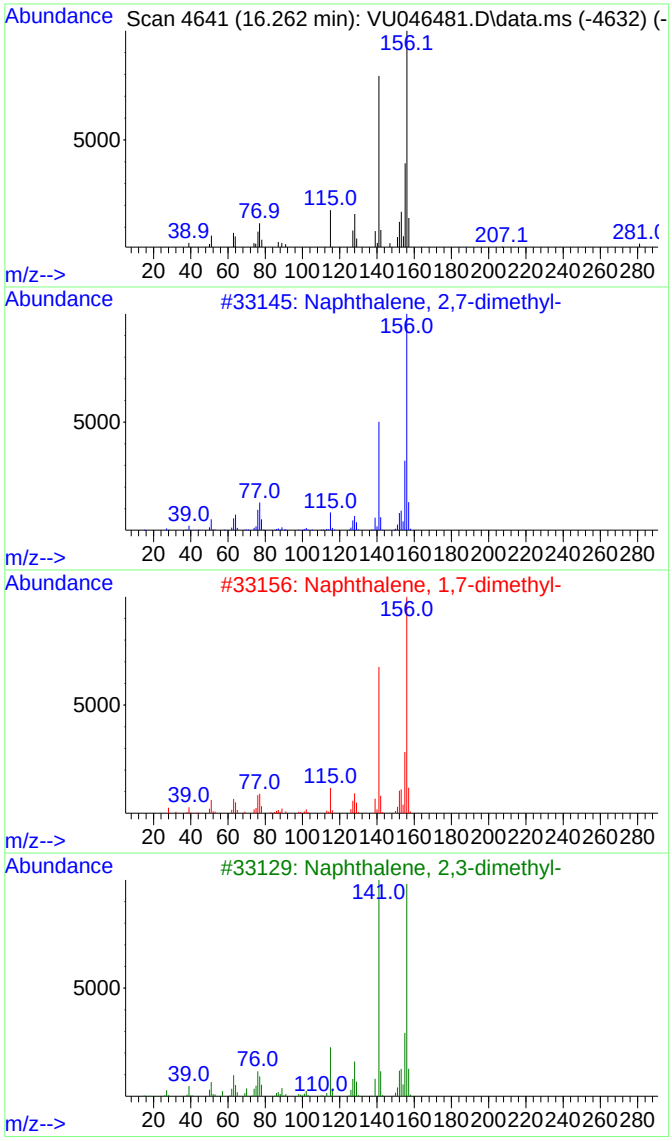
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

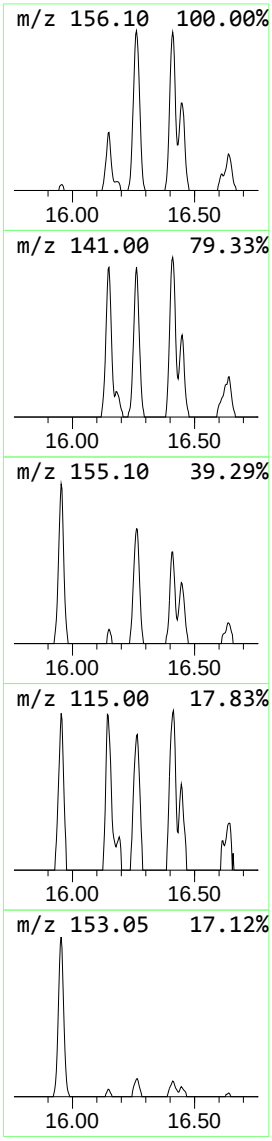
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Naphthalene, 2,7-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.262	3.80 ug/L	33727	1,4-Dichlorobenzene-d4	11.812

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
2	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
3	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	96
4	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
5	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	96





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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGL73

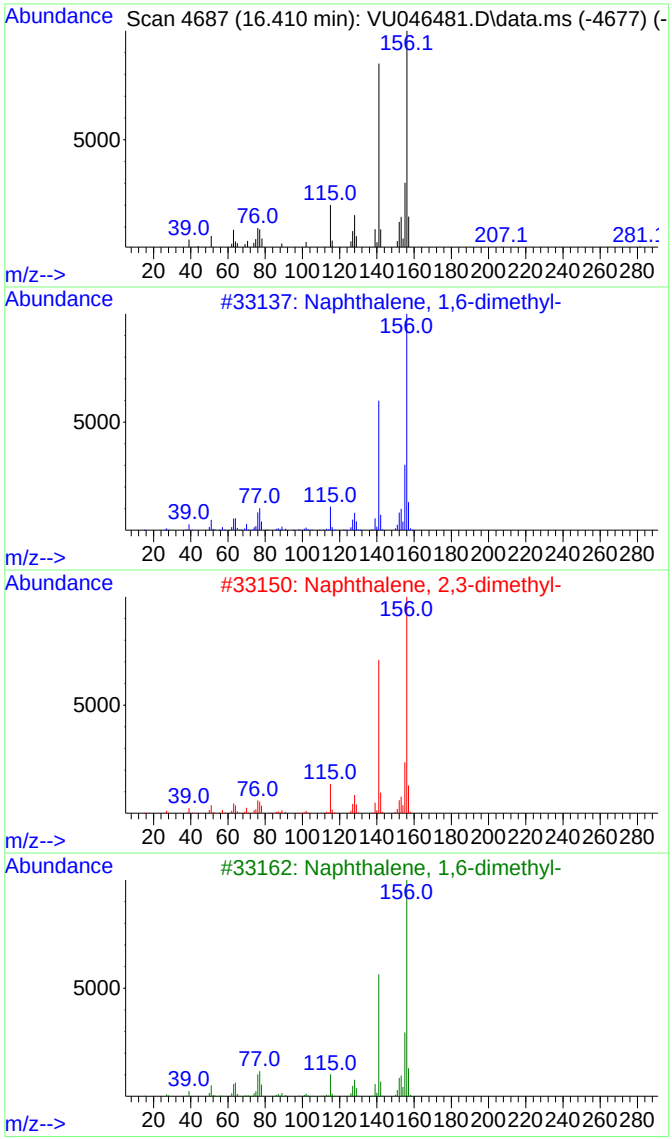
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

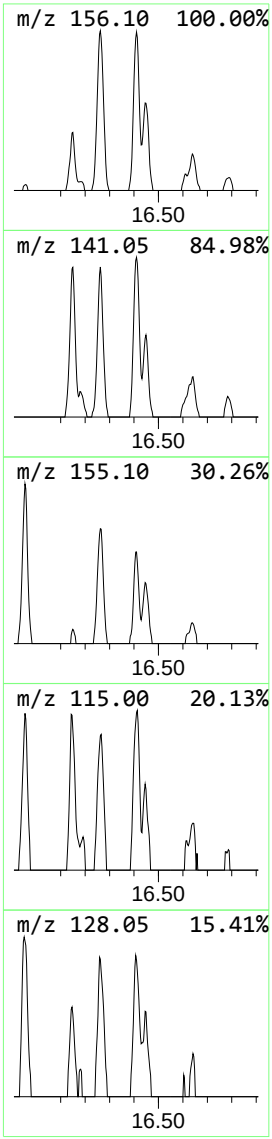
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Naphthalene, 1,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.410	3.34 ug/L	29638	1,4-Dichlorobenzene-d4	11.812

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
2	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
3	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
4	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	95
5	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	95





Tentatively Identified Compound (LSC) summary

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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGL73

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.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
Azulene	14.089	6.1	ug/L	53840	3	11.812	443297	50.0
Naphthalene, 2,...	16.262	3.8	ug/L	33727	3	11.812	443297	50.0
Naphthalene, 1,...	16.410	3.3	ug/L	29638	3	11.812	443297	50.0