

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
 Data File : VU048015.D
 Acq On : 13 Apr 2022 19:40
 Operator : SY/MD
 Sample : N2316-04ME
 Misc : 6.86g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNQ2ME

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\SFAMULM032422WMA.M
 Title : VOC Analysis

Signal : TIC: VU048015.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	72	80	117	rVB	123903	292692	4.28%	1.306%
2	1.893	167	172	181	rBV	57805	89099	1.30%	0.398%
3	2.539	358	373	387	rBV	371140	650262	9.51%	2.901%
4	2.845	463	468	470	rBV3	549	528	0.01%	0.002%
5	2.951	497	501	502	rBV3	1421	980	0.01%	0.004%
6	3.112	544	551	554	rVB4	865	989	0.01%	0.004%
7	3.427	644	649	653	rBV3	570	690	0.01%	0.003%
8	3.633	707	713	716	rBV2	577	499	0.01%	0.002%
9	3.681	724	728	733	rVV5	1278	1325	0.02%	0.006%
10	4.517	984	988	994	rVB3	646	637	0.01%	0.003%
11	4.642	1010	1027	1083	rBV	154246	570913	8.35%	2.547%
12	5.063	1140	1158	1185	rBV	356926	824416	12.06%	3.678%
13	5.356	1239	1249	1250	rBV3	918	1137	0.02%	0.005%
14	5.369	1250	1253	1260	rVV4	1742	1991	0.03%	0.009%
15	5.719	1341	1362	1397	rBV2	845713	2260507	33.07%	10.086%
16	5.880	1407	1412	1413	rBV5	609	551	0.01%	0.002%
17	5.980	1438	1443	1445	rBV3	934	775	0.01%	0.003%
18	6.124	1479	1488	1499	rBV5	2240	3680	0.05%	0.016%
19	6.247	1511	1526	1553	rBV	435311	873900	12.79%	3.899%
20	6.526	1604	1613	1626	rVB5	3208	6267	0.09%	0.028%
21	6.607	1631	1638	1644	rBV4	857	1302	0.02%	0.006%
22	6.690	1649	1664	1694	rBV	465801	970306	14.20%	4.329%
23	6.800	1695	1698	1709	rVV7	2629	3889	0.06%	0.017%
24	6.858	1709	1716	1724	rVB7	1537	2674	0.04%	0.012%
25	7.060	1769	1779	1781	rBV3	1424	1699	0.02%	0.008%
26	7.192	1807	1820	1843	rBV6	9038	28607	0.42%	0.128%
27	7.423	1883	1892	1903	rBV5	2564	4482	0.07%	0.020%
28	7.497	1903	1915	1922	rBV6	8733	17052	0.25%	0.076%
29	7.568	1925	1937	1956	rVB	232015	451156	6.60%	2.013%
30	7.899	2014	2040	2055	rBV	983043	1768074	25.87%	7.889%
31	7.970	2056	2062	2084	rVB2	25704	55335	0.81%	0.247%
32	8.128	2105	2111	2117	rBV3	4435	6012	0.09%	0.027%
33	8.182	2117	2128	2153	rVB	148134	315092	4.61%	1.406%
34	8.369	2177	2186	2201	rVB5	3379	7788	0.11%	0.035%
35	8.539	2233	2239	2243	rBV5	950	1102	0.02%	0.005%
36	8.584	2243	2253	2259	rBV7	1550	2636	0.04%	0.012%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
 Title : VOC Analysis

37	8.661	2259	2277	2316	rBV	653921	1365069	19.97%	6.090%
38	8.864	2334	2340	2346	rVB4	2243	2847	0.04%	0.013%
39	8.915	2352	2356	2359	rBV3	1456	1335	0.02%	0.006%
40	9.025	2383	2390	2391	rBV3	780	733	0.01%	0.003%
41	9.163	2428	2433	2435	rBV2	1276	1116	0.02%	0.005%
42	9.211	2445	2448	2454	rVB6	1015	1103	0.02%	0.005%
43	9.337	2479	2487	2488	rBV4	1183	1151	0.02%	0.005%
44	9.369	2492	2497	2500	rVV4	1257	1179	0.02%	0.005%
45	9.452	2500	2523	2552	rBV2	3020045	6834779	100.00%	30.494%
46	9.652	2581	2585	2586	rBV3	915	481	0.01%	0.002%
47	9.700	2592	2600	2609	rBV2	6106	10463	0.15%	0.047%
48	9.742	2611	2613	2622	rVB6	1986	2243	0.03%	0.010%
49	9.800	2627	2631	2633	rBV2	530	455	0.01%	0.002%
50	10.038	2699	2705	2706	rBV	583	555	0.01%	0.002%
51	10.105	2716	2726	2727	rBV5	3473	3426	0.05%	0.015%
52	10.275	2777	2779	2783	rVB3	809	461	0.01%	0.002%
53	10.346	2797	2801	2802	rBV3	1271	781	0.01%	0.003%
54	10.472	2834	2840	2842	rBV2	658	691	0.01%	0.003%
55	10.488	2842	2845	2852	rVB4	1127	969	0.01%	0.004%
56	10.668	2891	2901	2913	rBV5	6233	11201	0.16%	0.050%
57	10.767	2918	2932	2957	rVB	777230	1255788	18.37%	5.603%
58	10.861	2957	2961	2963	rBV5	901	734	0.01%	0.003%
59	10.999	2994	3004	3011	rVV6	4053	7499	0.11%	0.033%
60	11.066	3022	3025	3026	rBV3	853	514	0.01%	0.002%
61	11.105	3030	3037	3052	rVB9	4123	8945	0.13%	0.040%
62	11.298	3088	3097	3105	rBV10	2319	4988	0.07%	0.022%
63	11.378	3120	3122	3126	rVB2	880	630	0.01%	0.003%
64	11.420	3130	3135	3139	rVV5	1535	1627	0.02%	0.007%
65	11.468	3141	3150	3161	rVB4	7869	14831	0.22%	0.066%
66	11.574	3180	3183	3186	rBV4	1252	1059	0.02%	0.005%
67	11.642	3199	3204	3205	rBV3	756	585	0.01%	0.003%
68	11.713	3214	3226	3233	rBV10	5867	11195	0.16%	0.050%
69	11.816	3246	3258	3275	rBV	806815	1311472	19.19%	5.851%
70	11.960	3293	3303	3316	rVB9	5462	15524	0.23%	0.069%
71	12.102	3344	3347	3349	rBV4	660	506	0.01%	0.002%
72	12.198	3358	3377	3394	rBV	1107904	1805594	26.42%	8.056%
73	12.381	3430	3434	3436	rBV5	1884	1676	0.02%	0.007%
74	12.443	3450	3453	3458	rBV5	809	927	0.01%	0.004%
75	12.771	3548	3555	3563	rVB8	1903	3001	0.04%	0.013%
76	12.838	3564	3576	3583	rBV10	3479	6458	0.09%	0.029%

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 ClientSampleId :
 ETNQ2ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Min Area: 0 % of largest Peak

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Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
 Title : VOC Analysis

77	12.973	3601	3618	3630	rBV5	11234	21098	0.31%	0.094%
78	13.025	3631	3634	3635	rVV2	1063	665	0.01%	0.003%
79	13.053	3635	3643	3652	rVB10	4510	7583	0.11%	0.034%
80	13.111	3657	3661	3664	rBV4	1416	1356	0.02%	0.006%
81	13.224	3688	3696	3704	rBV4	7963	11210	0.16%	0.050%
82	13.285	3711	3715	3722	rVB6	2177	2693	0.04%	0.012%
83	13.340	3722	3732	3734	rBV6	4170	6420	0.09%	0.029%
84	13.561	3796	3801	3804	rBV2	1801	1972	0.03%	0.009%
85	13.587	3804	3809	3817	rVB7	4511	6526	0.10%	0.029%
86	13.841	3879	3888	3899	rBV5	8713	15589	0.23%	0.070%
87	13.963	3918	3926	3932	rBV8	2629	4602	0.07%	0.021%
88	14.169	3982	3990	3991	rBV6	3323	4215	0.06%	0.019%
89	14.250	4012	4015	4016	rBV4	797	451	0.01%	0.002%
90	14.369	4044	4052	4056	rBV10	4768	7344	0.11%	0.033%
91	14.494	4084	4091	4102	rVB6	17212	28579	0.42%	0.128%
92	14.571	4111	4115	4116	rBV4	3129	2233	0.03%	0.010%
93	14.661	4134	4143	4160	rBV8	23235	43701	0.64%	0.195%
94	14.758	4170	4173	4175	rBV4	1640	1103	0.02%	0.005%
95	14.941	4222	4230	4244	rVB4	6386	10985	0.16%	0.049%
96	15.015	4244	4253	4254	rBV7	6467	7139	0.10%	0.032%
97	15.118	4272	4285	4293	rBV4	21121	48864	0.71%	0.218%
98	15.346	4348	4356	4366	rBV3	31896	53815	0.79%	0.240%
99	15.545	4411	4418	4428	rVB3	38981	57555	0.84%	0.257%
100	16.391	4672	4681	4693	rBV4	76551	153905	2.25%	0.687%

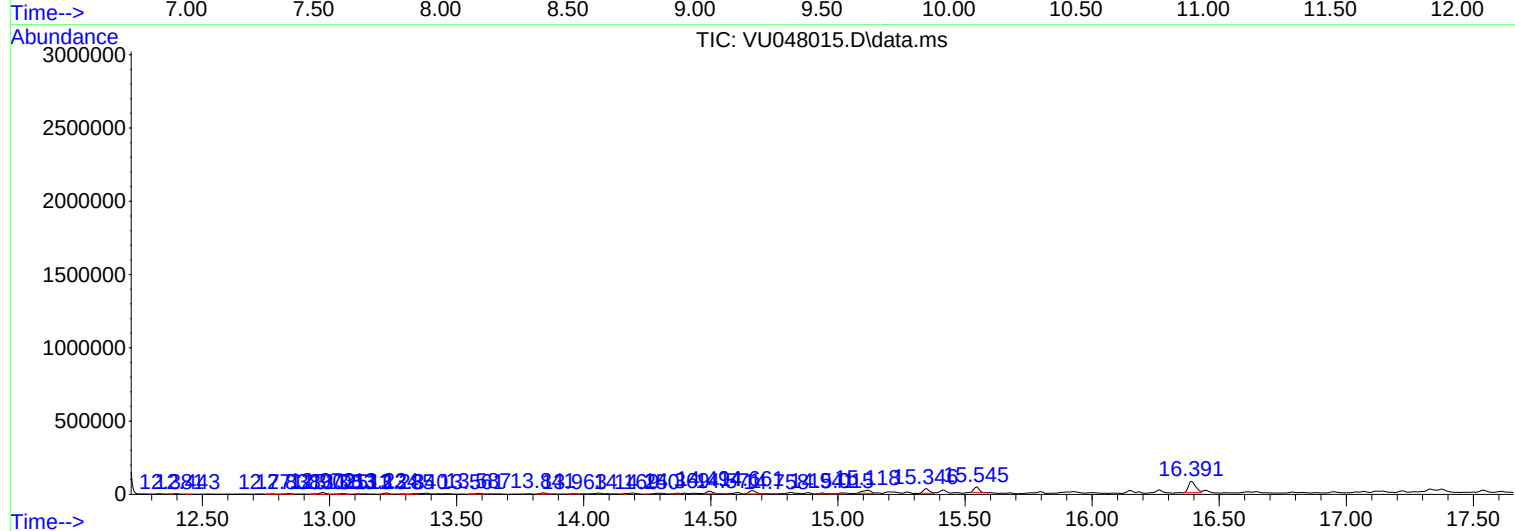
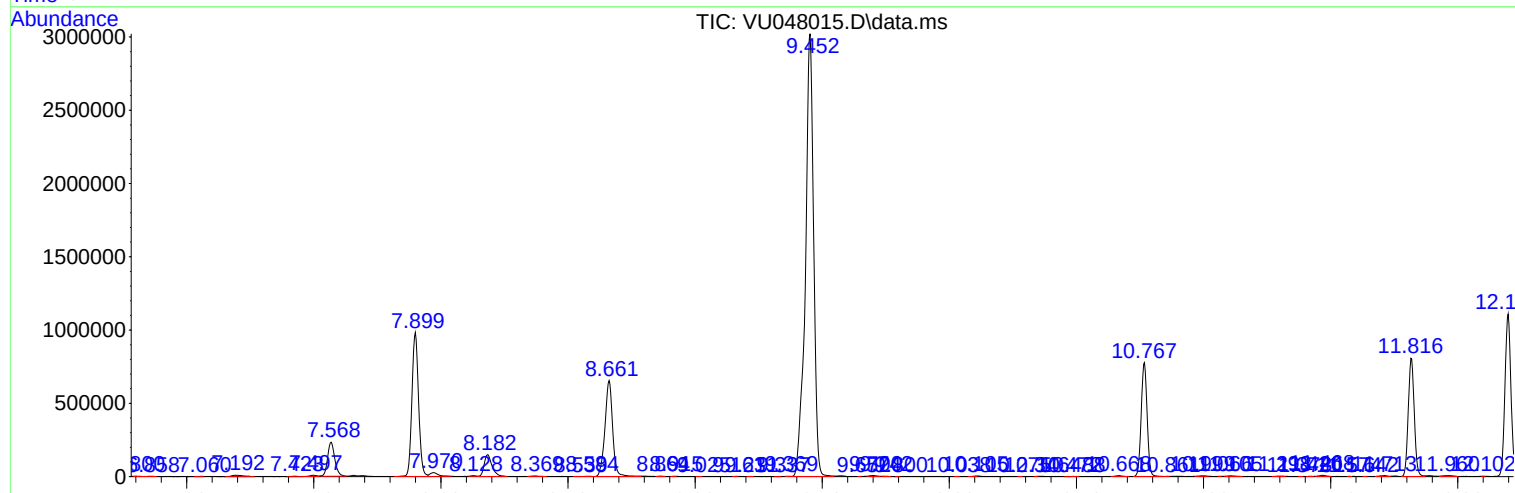
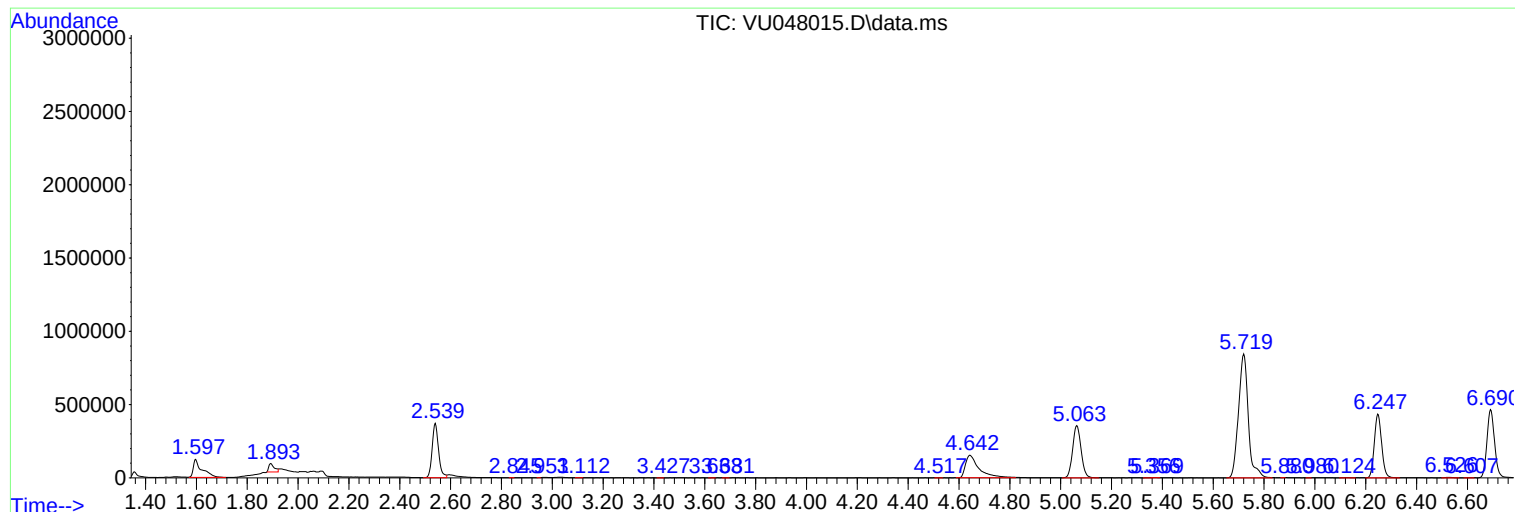
Sum of corrected areas: 22413238

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ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNQ2ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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



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Instrument :
MSVOA_U
ClientSampleId :
ETNQ2ME

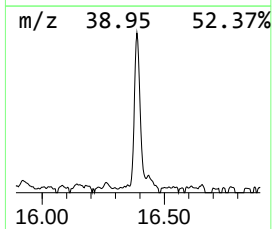
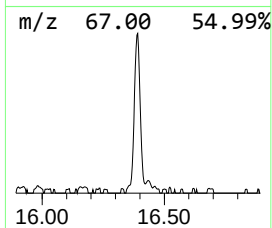
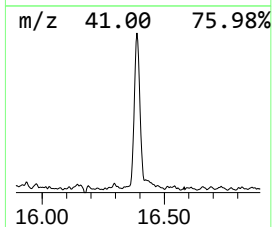
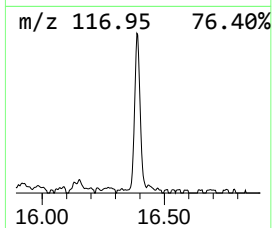
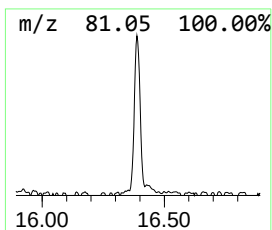
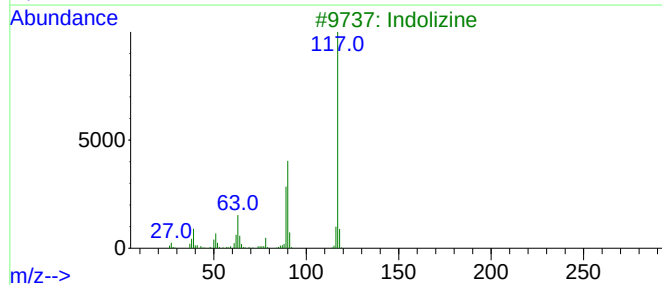
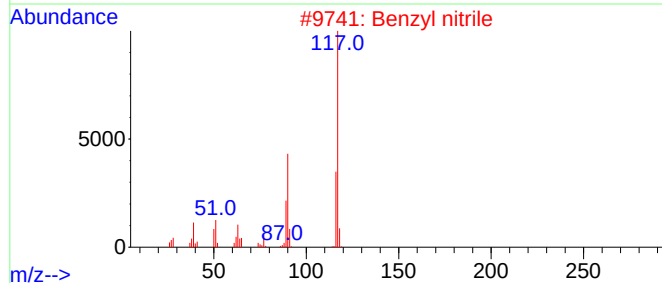
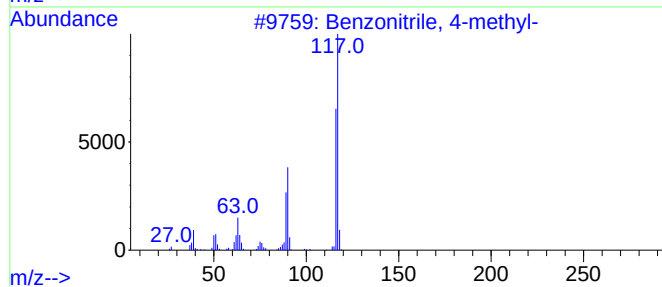
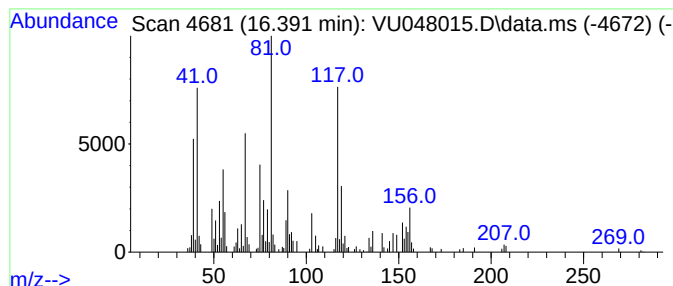
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.391	5.87 ug/L	153905	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzonitrile, 4-methyl-	117	C8H7N	000104-85-8	25
2			Benzyl nitrile	117	C8H7N	000140-29-4	25
3			Indolizine	117	C8H7N	000274-40-8	25
4			Benzyl nitrile	117	C8H7N	000140-29-4	25
5			Propane, 2-(methylthio)-	90	C4H10S	001551-21-9	22



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	16.391	5.9	ug/L	153905	3	11.819	1311470	50.0