

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100421\
 Data File : VU045106.D
 Acq On : 04 Oct 2021 19:05
 Operator : SY/MD
 Sample : M3974-09ME
 Misc : 5.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW8Z3ME

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\SFAMULM092321WMA.M
 Title : VOC Analysis

Signal : TIC: VU045106.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.469	33	40	52	rBV2	31997	62692	2.87%	0.476%
2	1.597	73	80	99	rVB	95544	145768	6.68%	1.106%
3	1.893	166	172	186	rBV	36616	59702	2.74%	0.453%
4	2.533	357	371	386	rBV	199842	350477	16.06%	2.659%
5	2.951	494	501	502	rBV2	500	432	0.02%	0.003%
6	2.967	503	506	512	rVB3	493	576	0.03%	0.004%
7	3.044	518	530	545	rVB7	3910	10430	0.48%	0.079%
8	3.109	545	550	558	rBV3	425	703	0.03%	0.005%
9	3.182	562	573	587	rVV2	1244	2905	0.13%	0.022%
10	3.337	608	621	636	rVB5	3400	7932	0.36%	0.060%
11	3.674	713	726	735	rBV4	2457	5368	0.25%	0.041%
12	4.051	833	843	846	rBV2	241	429	0.02%	0.003%
13	4.510	975	986	997	rVV4	3039	6728	0.31%	0.051%
14	4.662	1013	1033	1080	rBV2	194288	684781	31.38%	5.196%
15	5.067	1140	1159	1199	rBV	194112	485257	22.23%	3.682%
16	5.205	1199	1202	1207	rVB	354	324	0.01%	0.002%
17	5.292	1225	1229	1238	rVB3	550	824	0.04%	0.006%
18	5.375	1242	1255	1267	rBV6	4012	8959	0.41%	0.068%
19	5.584	1312	1320	1330	rBV4	974	1646	0.08%	0.012%
20	5.629	1330	1334	1340	rVB4	676	605	0.03%	0.005%
21	5.723	1341	1363	1386	rBV2	475923	1224015	56.08%	9.288%
22	5.845	1395	1401	1408	rVB3	1824	2773	0.13%	0.021%
23	5.909	1411	1421	1430	rVB7	1320	2314	0.11%	0.018%
24	5.983	1430	1444	1474	rVB4	10676	27399	1.26%	0.208%
25	6.124	1478	1488	1496	rVB5	2210	3930	0.18%	0.030%
26	6.250	1511	1527	1555	rBV	366437	757485	34.71%	5.748%
27	6.346	1555	1557	1562	rVB3	486	367	0.02%	0.003%
28	6.542	1593	1618	1650	rBV	1110235	2182462	100.00%	16.561%
29	6.694	1651	1665	1681	rBV	270845	569899	26.11%	4.324%
30	6.977	1741	1753	1760	rBV5	1439	2192	0.10%	0.017%
31	7.063	1770	1780	1792	rVV6	963	2042	0.09%	0.015%
32	7.195	1809	1821	1826	rBV5	2783	5855	0.27%	0.044%
33	7.395	1877	1883	1887	rBV2	834	1045	0.05%	0.008%
34	7.443	1891	1898	1900	rBV3	556	601	0.03%	0.005%
35	7.497	1907	1915	1921	rBV4	1220	1727	0.08%	0.013%
36	7.571	1924	1938	1961	rBV	140357	279992	12.83%	2.125%

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Instrument :
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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
 Title : VOC Analysis

37	7.687	1969	1974	1976	rBV4	928	911	0.04%	0.007%
38	7.758	1989	1996	2005	rVB7	1048	1596	0.07%	0.012%
39	7.903	2018	2041	2056	rBV	503554	934097	42.80%	7.088%
40	7.973	2057	2063	2074	rVB	9217	15813	0.72%	0.120%
41	8.099	2098	2102	2104	rVV2	675	484	0.02%	0.004%
42	8.128	2105	2111	2117	rVV4	2119	2667	0.12%	0.020%
43	8.185	2117	2129	2161	rVB	82855	190772	8.74%	1.448%
44	8.372	2178	2187	2193	rVB2	773	1194	0.05%	0.009%
45	8.555	2234	2244	2255	rVB3	11067	17684	0.81%	0.134%
46	8.671	2260	2280	2310	rBV	387774	854773	39.17%	6.486%
47	8.864	2333	2340	2351	rVB5	3067	4936	0.23%	0.037%
48	8.925	2351	2359	2366	rBV3	1684	2475	0.11%	0.019%
49	9.124	2416	2421	2425	rBV2	364	372	0.02%	0.003%
50	9.166	2429	2434	2438	rVV4	742	885	0.04%	0.007%
51	9.211	2442	2448	2457	rVB4	1323	1714	0.08%	0.013%
52	9.337	2481	2487	2497	rVB3	1553	2346	0.11%	0.018%
53	9.427	2499	2515	2534	rBV	445602	935641	42.87%	7.100%
54	9.578	2551	2562	2576	rVB	12161	22076	1.01%	0.168%
55	9.661	2582	2588	2589	rBV	493	530	0.02%	0.004%
56	9.703	2593	2601	2613	rVB5	5128	9635	0.44%	0.073%
57	9.893	2656	2660	2665	rVB2	436	319	0.01%	0.002%
58	10.034	2696	2704	2713	rVV4	1224	2312	0.11%	0.018%
59	10.111	2719	2728	2736	rBV3	3438	6185	0.28%	0.047%
60	10.256	2766	2773	2774	rBV4	1861	1784	0.08%	0.014%
61	10.359	2798	2805	2810	rBV5	2336	3461	0.16%	0.026%
62	10.491	2839	2846	2854	rVB3	4076	6949	0.32%	0.053%
63	10.565	2866	2869	2875	rVB6	627	510	0.02%	0.004%
64	10.629	2884	2889	2893	rVV2	1142	1204	0.06%	0.009%
65	10.671	2894	2902	2912	rVV5	2024	3924	0.18%	0.030%
66	10.771	2920	2933	2953	rBV	435995	721108	33.04%	5.472%
67	10.867	2959	2963	2967	rBV5	763	800	0.04%	0.006%
68	10.915	2969	2978	2988	rVB	7920	13145	0.60%	0.100%
69	11.005	2998	3006	3021	rBV4	4734	11972	0.55%	0.091%
70	11.095	3027	3034	3050	rVB2	10052	18897	0.87%	0.143%
71	11.301	3087	3098	3109	rBV	31381	50317	2.31%	0.382%
72	11.417	3129	3134	3142	rBV4	2991	4356	0.20%	0.033%
73	11.475	3143	3152	3167	rVB3	12195	22097	1.01%	0.168%
74	11.574	3177	3183	3185	rBV3	1112	1054	0.05%	0.008%
75	11.648	3201	3206	3214	rVB3	4606	6812	0.31%	0.052%
76	11.713	3215	3226	3232	rBV7	2907	6035	0.28%	0.046%

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 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW8Z3ME

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\SFAMULM092321WMA.M
 Title : VOC Analysis

77	11.748	3232	3237	3246	rVB3	6786	9947	0.46%	0.075%
78	11.822	3246	3260	3273	rBV	571504	900992	41.28%	6.837%
79	12.102	3337	3347	3364	rVV3	34353	65054	2.98%	0.494%
80	12.201	3364	3378	3396	rVB	554314	903850	41.41%	6.859%
81	12.308	3408	3411	3413	rBV3	2043	1472	0.07%	0.011%
82	12.381	3428	3434	3449	rVB2	5220	9019	0.41%	0.068%
83	12.471	3454	3462	3467	rBV3	8475	12570	0.58%	0.095%
84	12.578	3487	3495	3502	rBV	16480	22765	1.04%	0.173%
85	12.619	3503	3508	3516	rVB	7128	8921	0.41%	0.068%
86	12.687	3519	3529	3550	rVB3	32621	68511	3.14%	0.520%
87	12.816	3562	3569	3575	rBV6	2585	4551	0.21%	0.035%
88	12.877	3584	3588	3599	rVB3	7687	12173	0.56%	0.092%
89	13.115	3657	3662	3664	rBV6	3933	3748	0.17%	0.028%
90	13.298	3712	3719	3731	rVB2	15938	23248	1.07%	0.176%
91	13.455	3758	3768	3784	rVB3	82754	145408	6.66%	1.103%
92	13.738	3850	3856	3862	rBV5	3811	4508	0.21%	0.034%
93	13.790	3864	3872	3879	rVB2	10998	16746	0.77%	0.127%
94	13.841	3881	3888	3901	rVV6	8412	14621	0.67%	0.111%
95	14.208	3991	4002	4013	rVB2	16451	34966	1.60%	0.265%
96	14.491	4085	4090	4096	rVB6	4440	4599	0.21%	0.035%
97	14.880	4206	4211	4222	rVB6	8624	13049	0.60%	0.099%
98	15.024	4249	4256	4264	rBV6	7527	10219	0.47%	0.078%
99	15.413	4368	4377	4399	rVB2	41449	84596	3.88%	0.642%
100	15.979	4548	4553	4567	rVB	13669	18386	0.84%	0.140%

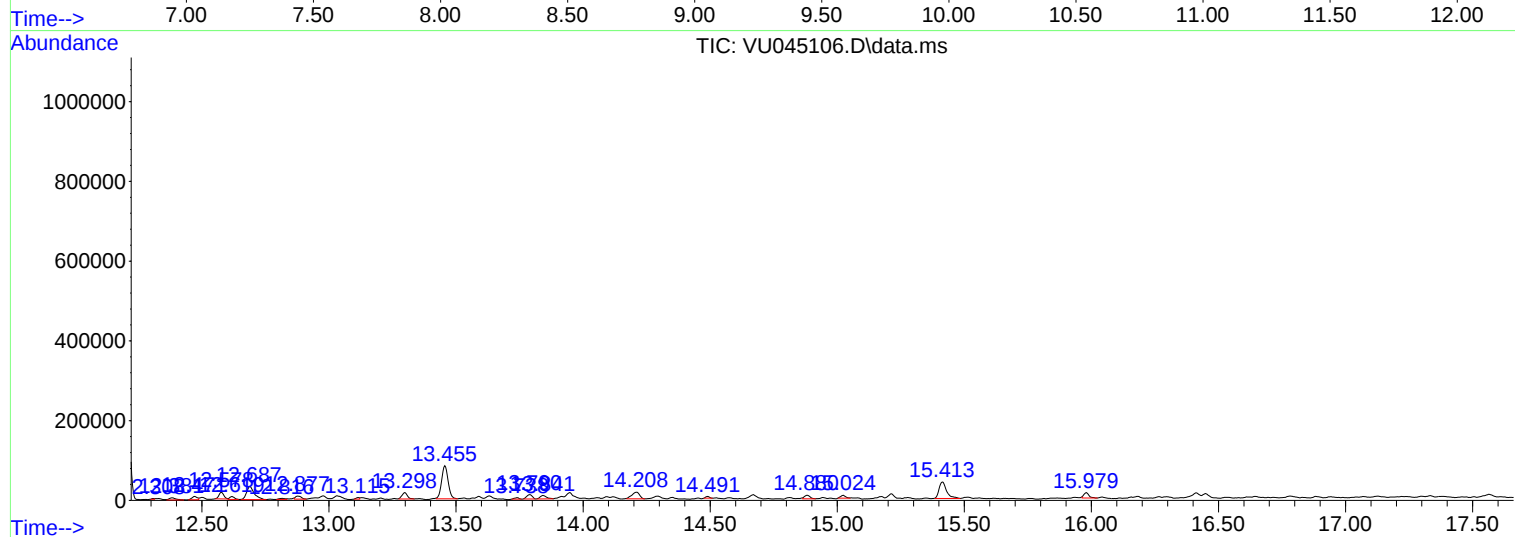
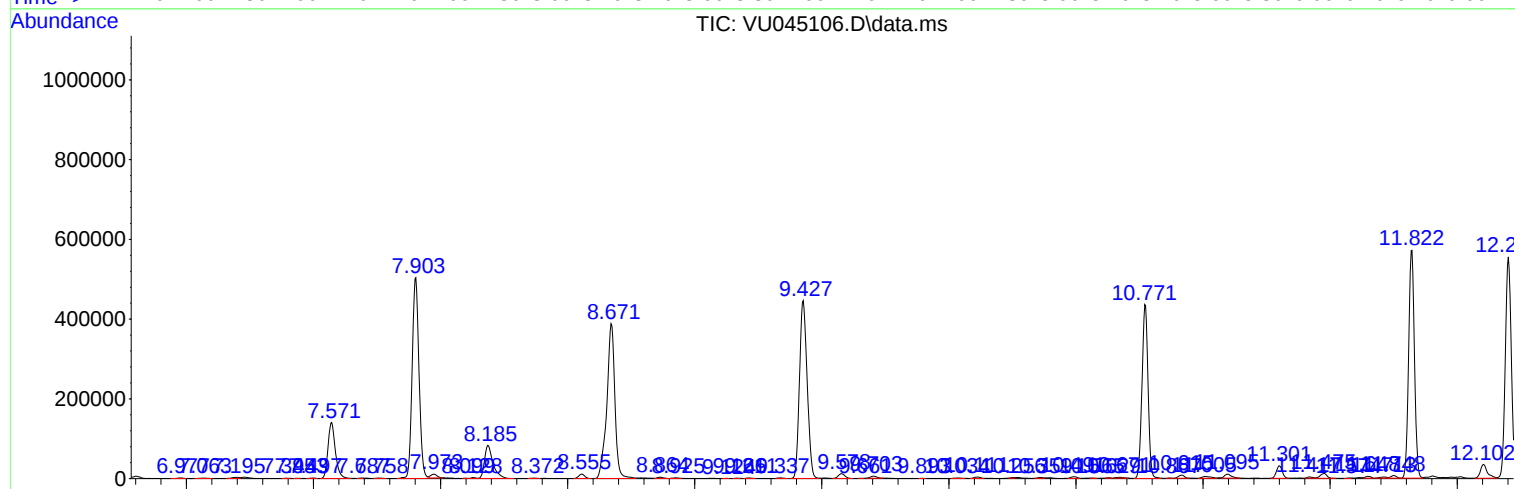
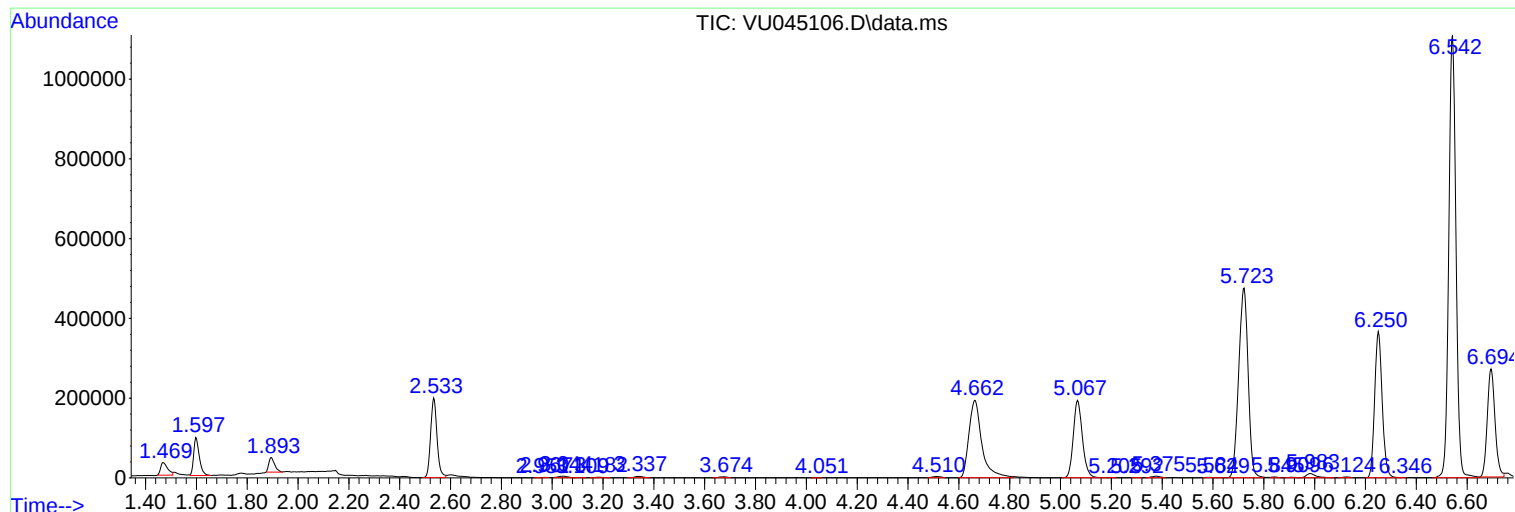
Sum of corrected areas: 13178397

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Misc : 5.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW8Z3ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW8Z3ME

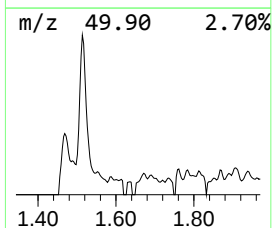
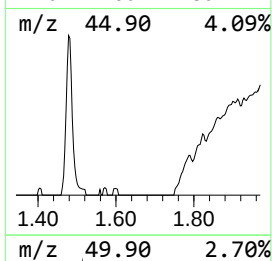
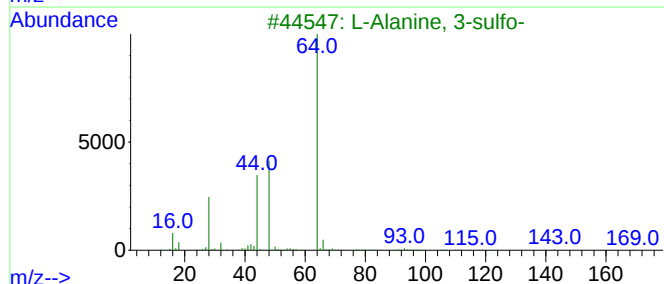
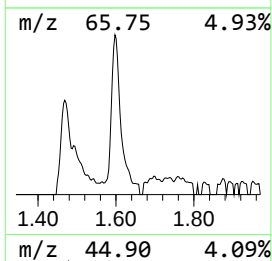
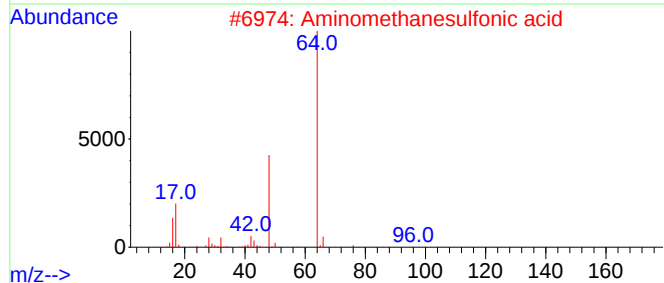
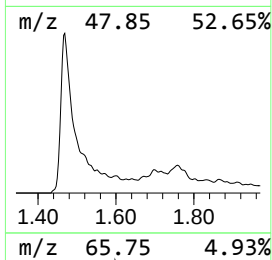
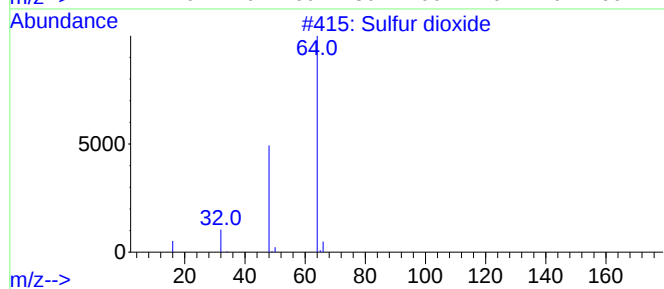
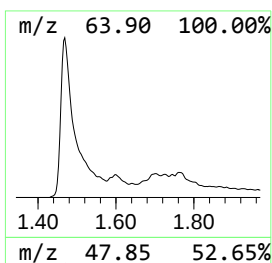
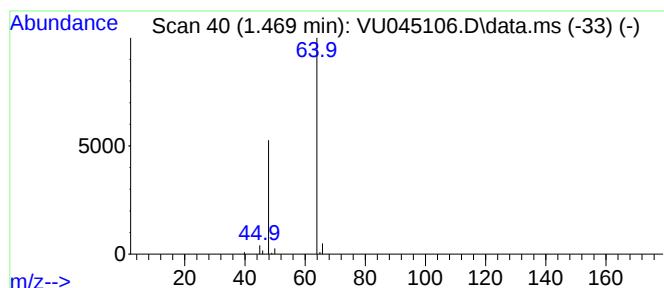
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.469	4.14 ug/L	62692	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
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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Instrument :
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ClientSampleId :
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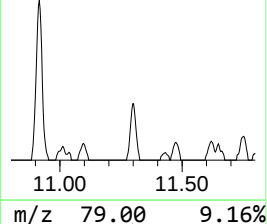
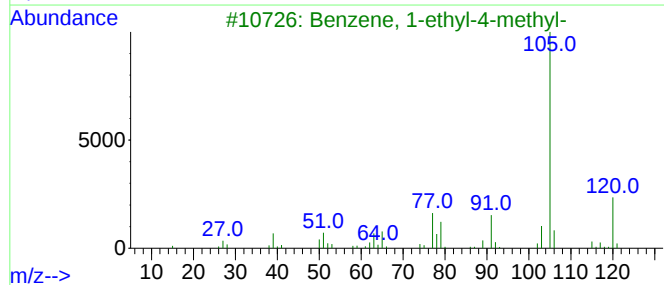
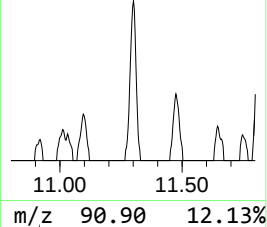
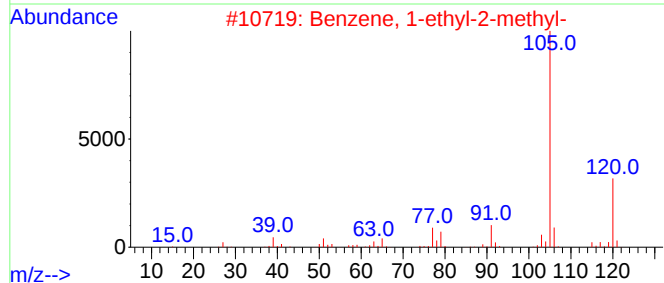
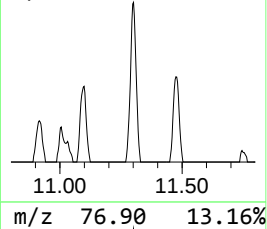
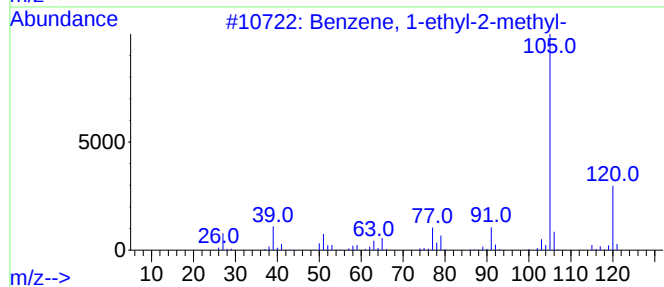
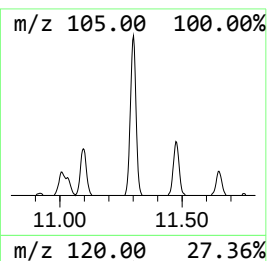
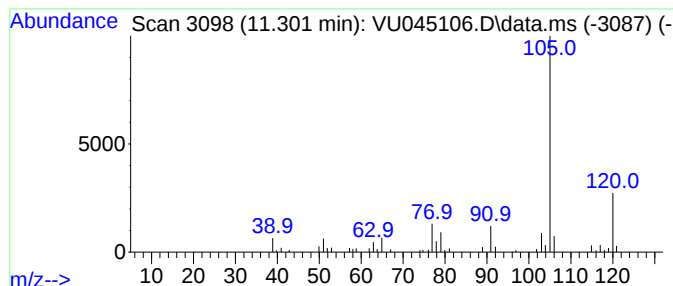
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Benzene, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.301	2.79 ug/L	50317	1,4-Dichlorobenzene-d4	11.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Mesitylene	120	C9H12	000108-67-8	91



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Instrument :
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ClientSampleId :
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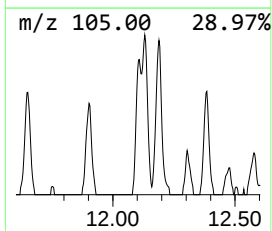
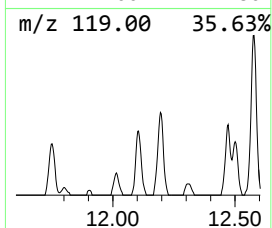
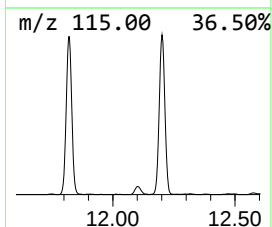
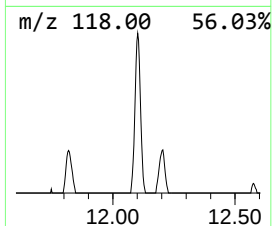
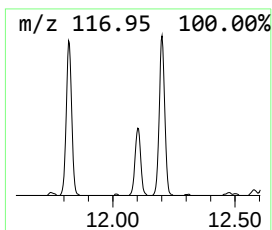
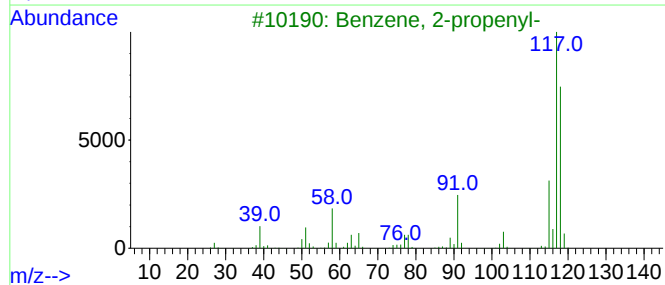
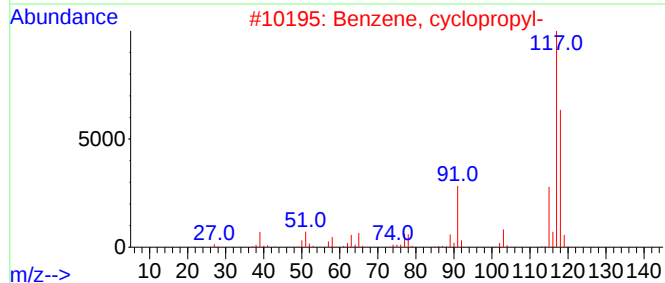
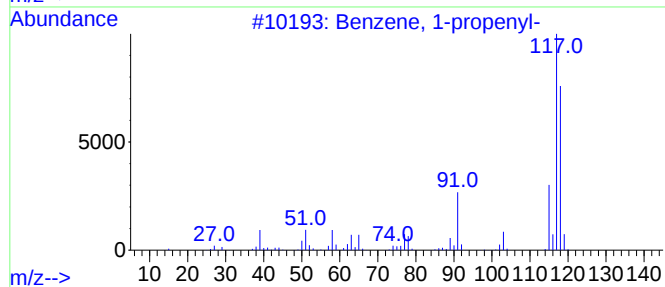
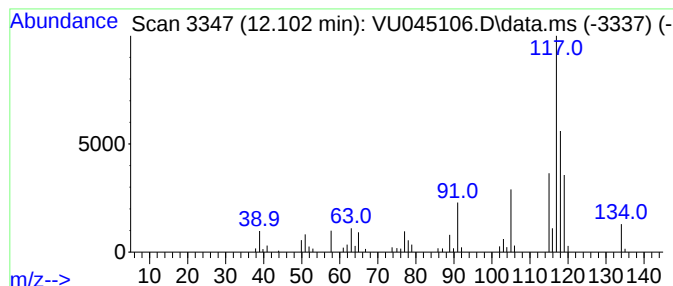
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Quant Title : VOC Analysis

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

Peak Number 4 Benzene, 1-propenyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.102	3.61 ug/L	65054	1,4-Dichlorobenzene-d4	11.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-propenyl-	118	C9H10	000637-50-3	93
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	70
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	70
4			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	70
5			Indane	118	C9H10	000496-11-7	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100421\
Data File : VU045106.D
Acq On : 04 Oct 2021 19:05
Operator : SY/MD
Sample : M3974-09ME
Misc : 5.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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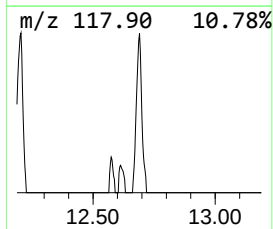
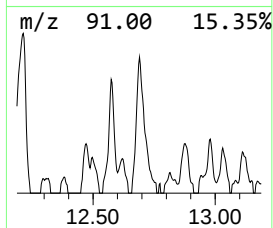
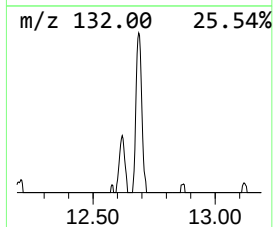
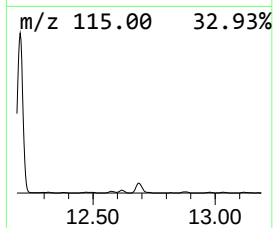
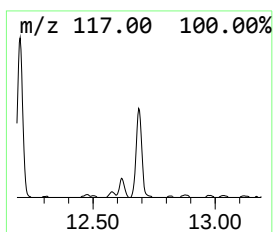
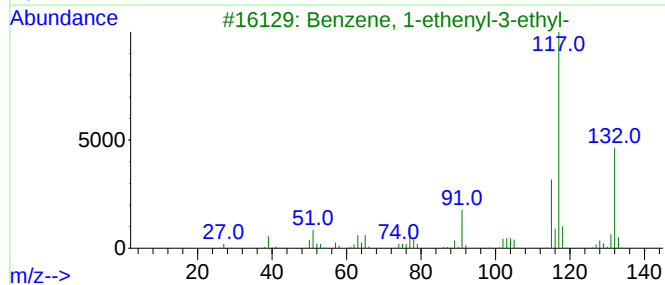
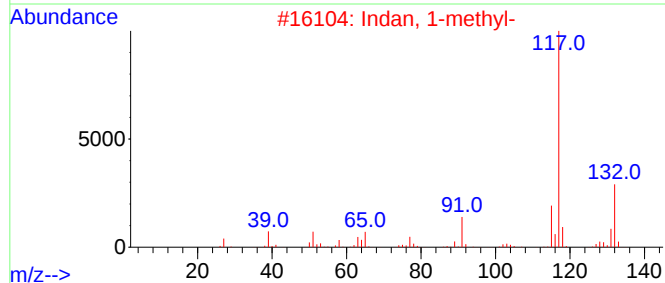
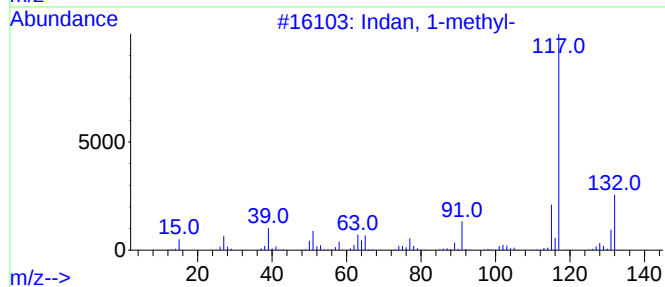
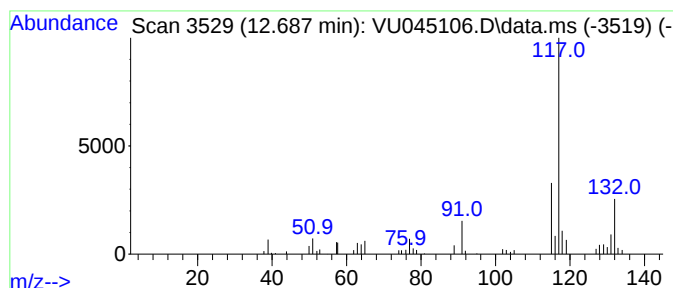
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Quant Title : VOC Analysis

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

Peak Number 5 Indan, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.687	3.80 ug/L	68511	1,4-Dichlorobenzene-d4	11.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indan, 1-methyl-	132	C10H12	000767-58-8	87
2			Indan, 1-methyl-	132	C10H12	000767-58-8	87
3			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	86
4			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	83
5			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100421\
Data File : VU045106.D
Acq On : 04 Oct 2021 19:05
Operator : SY/MD
Sample : M3974-09ME
Misc : 5.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW8Z3ME

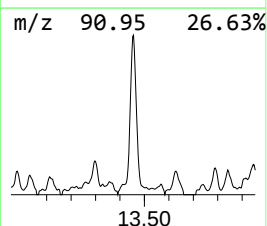
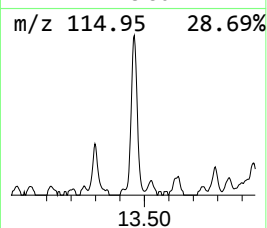
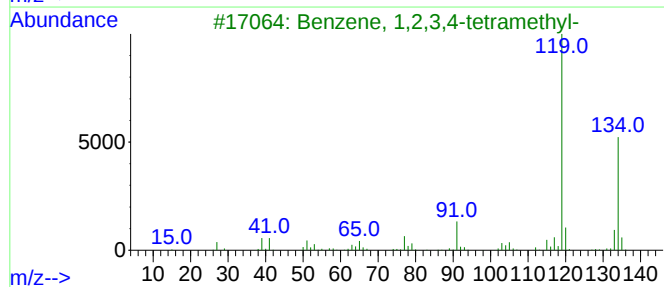
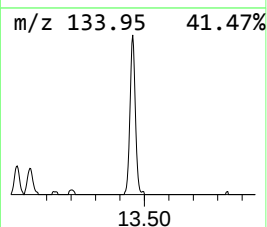
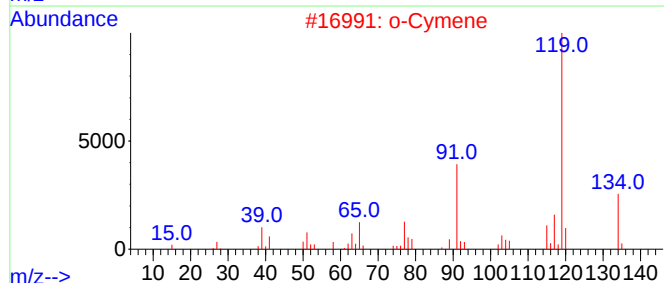
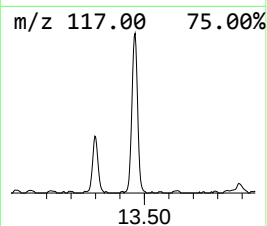
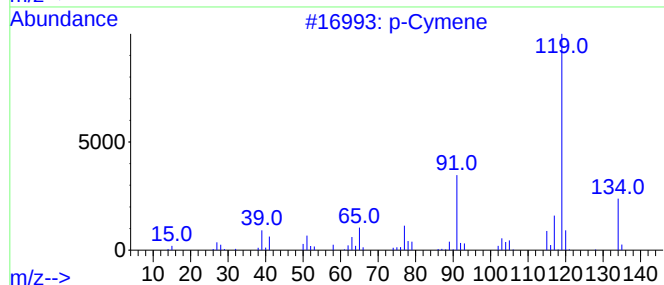
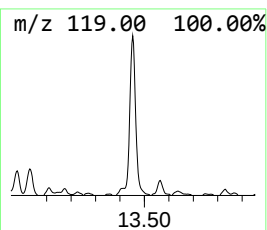
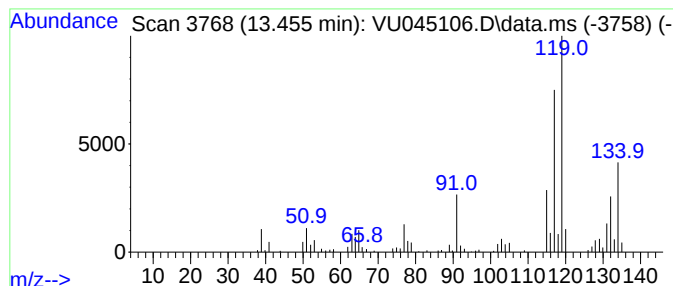
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Quant Title : VOC Analysis

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

Peak Number 6 p-Cymene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.455	8.07 ug/L	145408	1,4-Dichlorobenzene-d4	11.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			p-Cymene	134	C10H14	000099-87-6	55
2			o-Cymene	134	C10H14	000527-84-4	55
3			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	55
4			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	50
5			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100421\
Data File : VU045106.D
Acq On : 04 Oct 2021 19:05
Operator : SY/MD
Sample : M3974-09ME
Misc : 5.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW8Z3ME

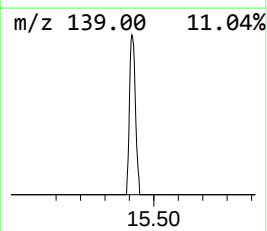
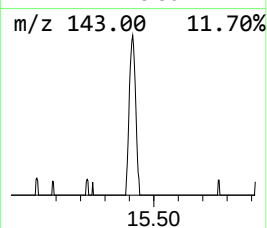
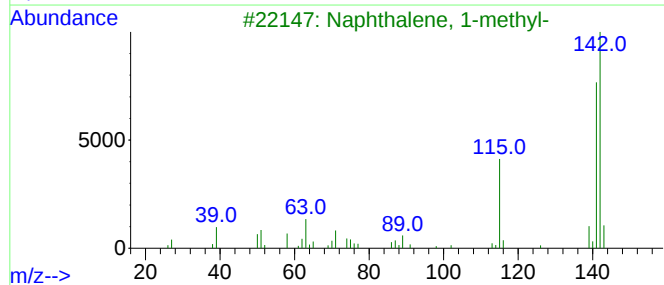
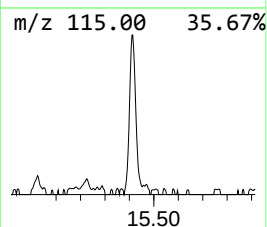
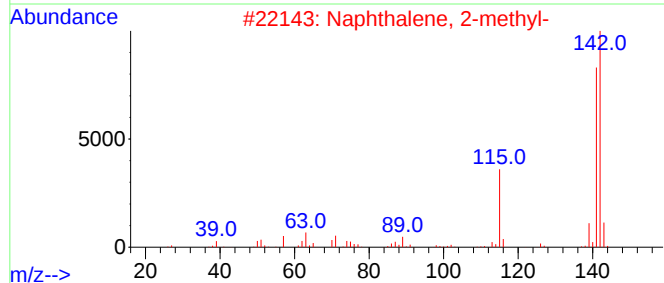
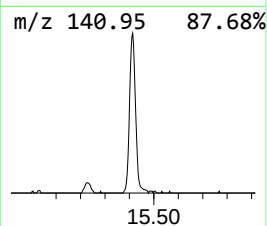
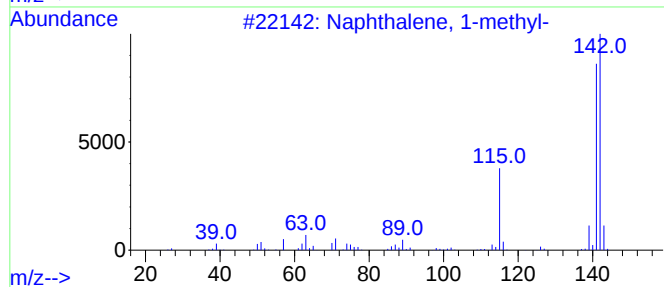
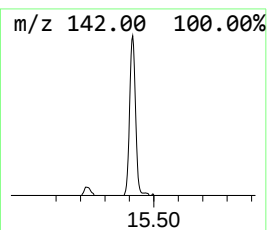
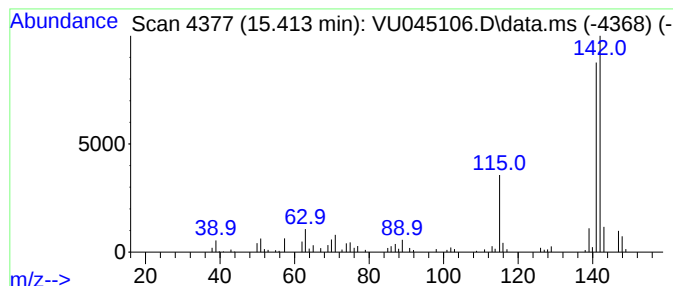
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Quant Title : VOC Analysis

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

Peak Number 7 Naphthalene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.414	4.69 ug/L	84596	1,4-Dichlorobenzene-d4	11.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	95
4			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	95
5			Benzocycloheptatriene	142	C11H10	000264-09-5	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100421\
Data File : VU045106.D
Acq On : 04 Oct 2021 19:05
Operator : SY/MD
Sample : M3974-09ME
Misc : 5.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW8Z3ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.469	4.1	ug/L	62692	1	6.250	757485	50.0
Benzene, 1-ethy...	11.301	2.8	ug/L	50317	3	11.822	900992	50.0
Benzene, 1-prop...	12.102	3.6	ug/L	65054	3	11.822	900992	50.0
Indan, 1-methyl-	12.687	3.8	ug/L	68511	3	11.822	900992	50.0
p-Cymene	13.455	8.1	ug/L	145408	3	11.822	900992	50.0
Naphthalene, 1-...	15.414	4.7	ug/L	84596	3	11.822	900992	50.0