

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100621\
 Data File : VU045192.D
 Acq On : 06 Oct 2021 17:48
 Operator : SY/MD
 Sample : M3973-03ME
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW8W9ME

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: VU0451192.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.456	29	36	51	rBV	93013	139385	9.49%	1.170%
2	1.597	72	80	98	rVB	166533	222923	15.18%	1.872%
3	1.871	160	165	180	rVB	53046	68969	4.70%	0.579%
4	2.520	353	367	387	rBV	271193	480263	32.71%	4.032%
5	2.742	431	436	449	rVB3	730	1214	0.08%	0.010%
6	2.790	449	451	455	rVB2	192	122	0.01%	0.001%
7	2.838	464	466	472	rVB2	182	176	0.01%	0.001%
8	2.874	472	477	481	rBV	342	344	0.02%	0.003%
9	2.919	488	491	495	rBV3	189	135	0.01%	0.001%
10	2.970	497	507	515	rVV5	767	1528	0.10%	0.013%
11	3.031	515	526	541	rVV4	4919	10905	0.74%	0.092%
12	3.186	560	574	587	rBV3	1588	4063	0.28%	0.034%
13	3.276	599	602	607	rBV2	146	146	0.01%	0.001%
14	3.514	671	676	679	rVB	252	194	0.01%	0.002%
15	3.581	694	697	701	rBV2	168	178	0.01%	0.001%
16	3.665	714	723	732	rVV3	935	1553	0.11%	0.013%
17	3.719	736	740	742	rVV2	163	147	0.01%	0.001%
18	3.735	742	745	750	rVV2	204	216	0.01%	0.002%
19	3.761	750	753	755	rVV2	209	142	0.01%	0.001%
20	3.777	755	758	762	rVB2	229	181	0.01%	0.002%
21	3.819	768	771	775	rVB	162	115	0.01%	0.001%
22	3.883	787	791	794	rBV2	197	166	0.01%	0.001%
23	4.051	839	843	846	rVB2	229	178	0.01%	0.001%
24	4.083	851	853	856	rBV2	171	120	0.01%	0.001%
25	4.182	881	884	885	rBV2	201	124	0.01%	0.001%
26	4.420	955	958	966	rBV2	326	477	0.03%	0.004%
27	4.546	992	997	999	rBV	238	249	0.02%	0.002%
28	4.649	1012	1029	1072	rVV	112071	368592	25.10%	3.095%
29	4.880	1097	1101	1106	rBV2	470	481	0.03%	0.004%
30	5.067	1140	1159	1185	rVV	234639	553601	37.70%	4.648%
31	5.163	1187	1189	1192	rVB2	225	130	0.01%	0.001%
32	5.195	1196	1199	1205	rVB3	526	429	0.03%	0.004%
33	5.253	1213	1217	1221	rBV2	143	127	0.01%	0.001%
34	5.295	1221	1230	1239	rVB3	671	1381	0.09%	0.012%
35	5.337	1240	1243	1248	rBV	147	132	0.01%	0.001%
36	5.719	1338	1362	1391	rBV2	587901	1468401	100.00%	12.328%

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Instrument :
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 ClientSampleId :
 EW8W9ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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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

37	5.919	1418	1424	1428	rVV2	173	178	0.01%	0.001%
38	5.983	1432	1444	1468	rVB4	9098	22805	1.55%	0.191%
39	6.108	1477	1483	1485	rBV2	187	187	0.01%	0.002%
40	6.250	1511	1527	1546	rBV	441317	881693	60.04%	7.402%
41	6.423	1577	1581	1583	rBV	184	157	0.01%	0.001%
42	6.530	1605	1614	1625	rVV7	4670	8784	0.60%	0.074%
43	6.607	1629	1638	1650	rVV3	4162	9325	0.64%	0.078%
44	6.694	1650	1665	1693	rVV	324824	670732	45.68%	5.631%
45	6.796	1693	1697	1699	rVV2	522	527	0.04%	0.004%
46	6.809	1699	1701	1707	rVV2	786	867	0.06%	0.007%
47	6.845	1710	1712	1716	rVB	244	176	0.01%	0.001%
48	6.951	1742	1745	1750	rVV2	152	134	0.01%	0.001%
49	7.038	1770	1772	1774	rBV	256	172	0.01%	0.001%
50	7.060	1777	1779	1782	rVB2	362	193	0.01%	0.002%
51	7.112	1792	1795	1798	rBV2	157	146	0.01%	0.001%
52	7.192	1813	1820	1825	rBV4	1373	2247	0.15%	0.019%
53	7.324	1858	1861	1864	rVB	204	139	0.01%	0.001%
54	7.401	1881	1885	1888	rVB	252	226	0.02%	0.002%
55	7.420	1888	1891	1892	rBV	219	127	0.01%	0.001%
56	7.430	1892	1894	1900	rVV2	122	145	0.01%	0.001%
57	7.497	1910	1915	1921	rVB4	612	683	0.05%	0.006%
58	7.571	1923	1938	1957	rBV	175793	336700	22.93%	2.827%
59	7.684	1969	1973	1974	rBV	347	254	0.02%	0.002%
60	7.777	1999	2002	2006	rBV2	273	240	0.02%	0.002%
61	7.902	2025	2041	2056	rBV	645849	1177204	80.17%	9.883%
62	7.973	2056	2063	2084	rVB2	9350	19417	1.32%	0.163%
63	8.131	2105	2112	2117	rBV2	868	838	0.06%	0.007%
64	8.185	2117	2129	2148	rVV	116670	225307	15.34%	1.892%
65	8.359	2179	2183	2184	rBV3	328	209	0.01%	0.002%
66	8.558	2242	2245	2249	rVB3	466	268	0.02%	0.002%
67	8.652	2259	2274	2306	rBV	433310	831467	56.62%	6.981%
68	8.922	2353	2358	2367	rBV5	873	1470	0.10%	0.012%
69	9.082	2404	2408	2410	rBV2	298	227	0.02%	0.002%
70	9.150	2427	2429	2434	rBV2	288	258	0.02%	0.002%
71	9.333	2480	2486	2490	rBV2	732	862	0.06%	0.007%
72	9.423	2500	2514	2538	rBV	598684	1100880	74.97%	9.242%
73	9.571	2554	2560	2562	rBV5	737	588	0.04%	0.005%
74	9.626	2573	2577	2578	rBV2	154	132	0.01%	0.001%
75	9.655	2583	2586	2590	rVV3	418	314	0.02%	0.003%
76	9.700	2590	2600	2606	rVV3	2167	3804	0.26%	0.032%

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Instrument :
 MSVOA_U
 ClientSampleId :
 EW8W9ME

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	9.748	2610	2615	2622	rVB3	1670	2164	0.15%	0.018%
78	9.890	2654	2659	2662	rVV4	333	389	0.03%	0.003%
79	9.909	2662	2665	2671	rVB2	242	214	0.01%	0.002%
80	9.935	2671	2673	2677	rBV2	178	138	0.01%	0.001%
81	9.957	2677	2680	2684	rVB2	179	122	0.01%	0.001%
82	10.018	2693	2699	2702	rBV4	634	707	0.05%	0.006%
83	10.066	2712	2714	2718	rBV	359	245	0.02%	0.002%
84	10.108	2722	2727	2733	rBV3	1000	1146	0.08%	0.010%
85	10.253	2760	2772	2781	rBV7	2027	4682	0.32%	0.039%
86	10.336	2795	2798	2799	rBV2	538	313	0.02%	0.003%
87	10.513	2849	2853	2854	rBV2	590	436	0.03%	0.004%
88	10.533	2854	2859	2864	rVV4	1305	1507	0.10%	0.013%
89	10.629	2883	2889	2893	rBV7	1653	2035	0.14%	0.017%
90	10.674	2895	2903	2914	rVB2	8535	14159	0.96%	0.119%
91	10.764	2919	2931	2955	rBV	473006	786322	53.55%	6.602%
92	11.118	3034	3041	3049	rBV2	9424	13836	0.94%	0.116%
93	11.420	3128	3135	3142	rBV2	9317	12578	0.86%	0.106%
94	11.462	3142	3148	3158	rVB4	7837	12751	0.87%	0.107%
95	11.819	3247	3259	3272	rBV	690928	1092579	74.41%	9.173%
96	12.198	3365	3377	3393	rVB	661624	1062132	72.33%	8.917%
97	12.330	3411	3418	3428	rVB	33893	46121	3.14%	0.387%
98	13.433	3754	3761	3769	rBV	61213	86087	5.86%	0.723%
99	13.590	3803	3810	3825	rVB2	38145	56244	3.83%	0.472%
100	14.452	4071	4078	4086	rVB	66165	86698	5.90%	0.728%

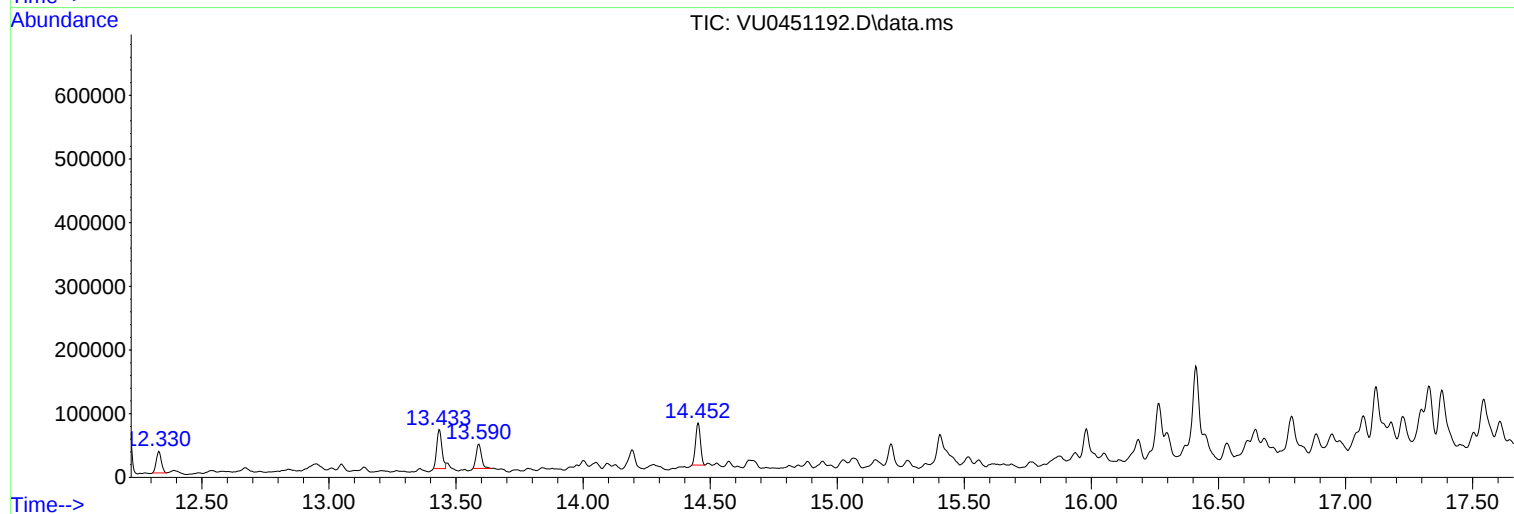
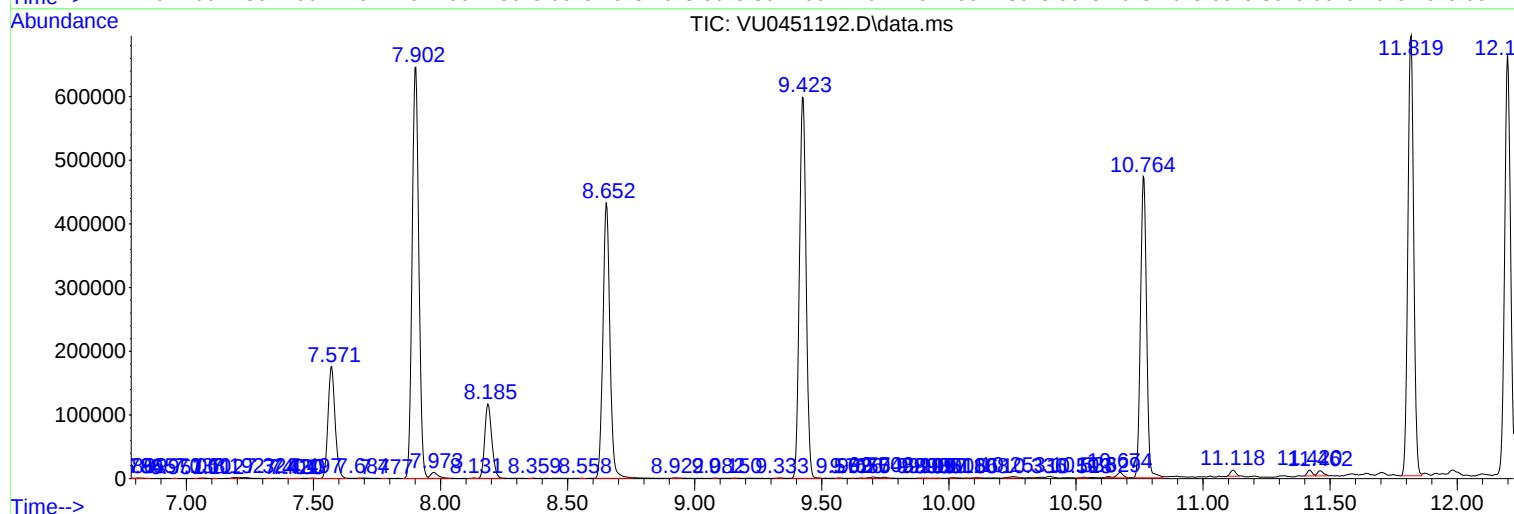
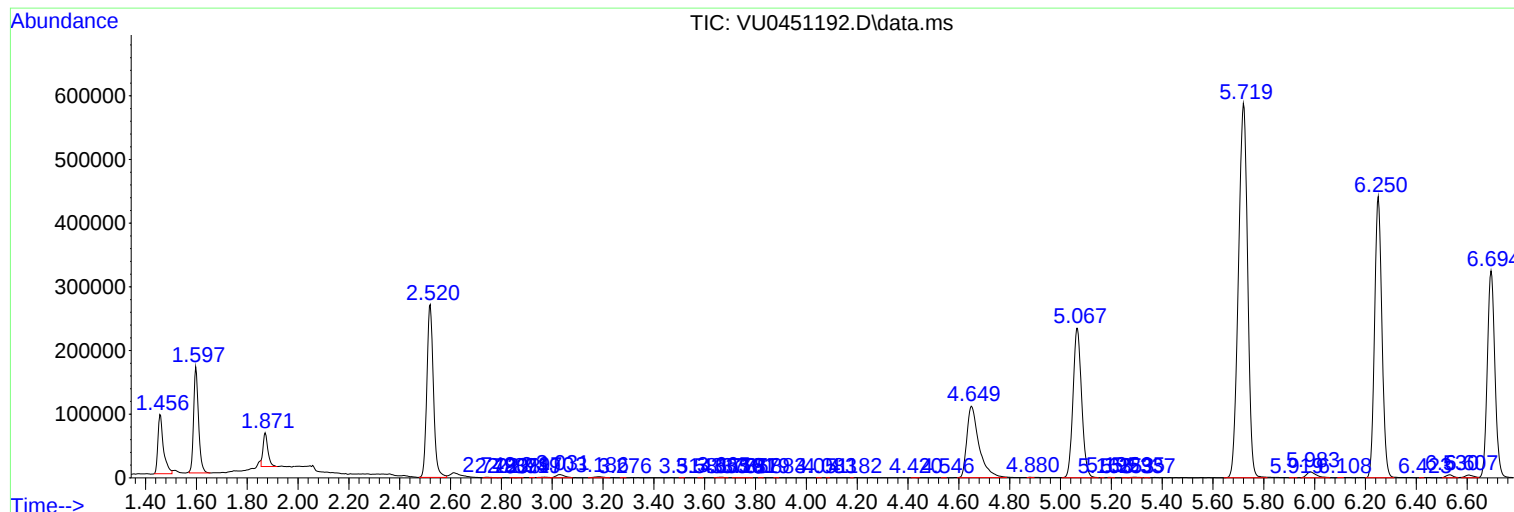
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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW8W9ME

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 : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW8W9ME

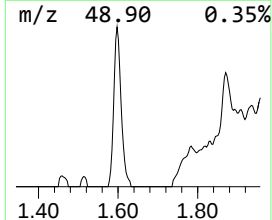
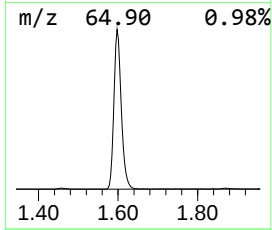
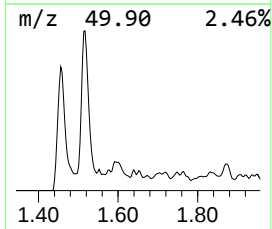
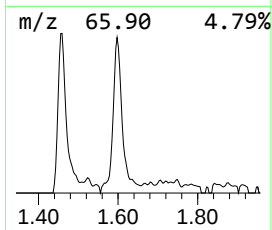
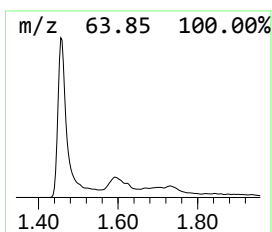
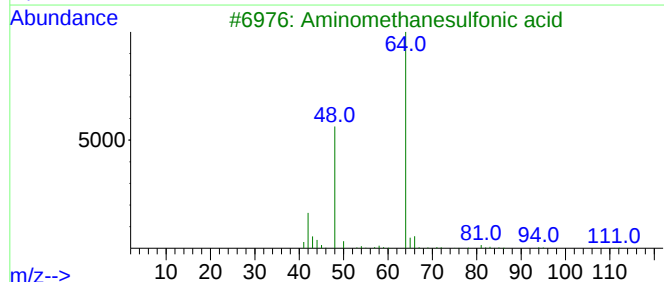
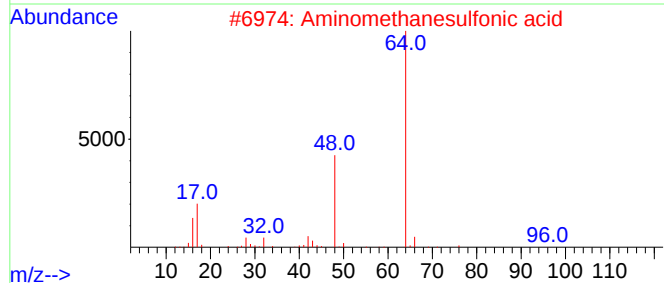
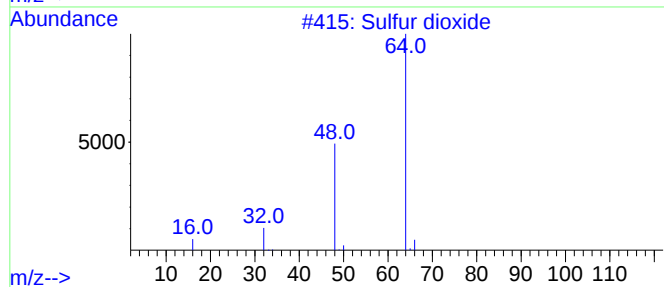
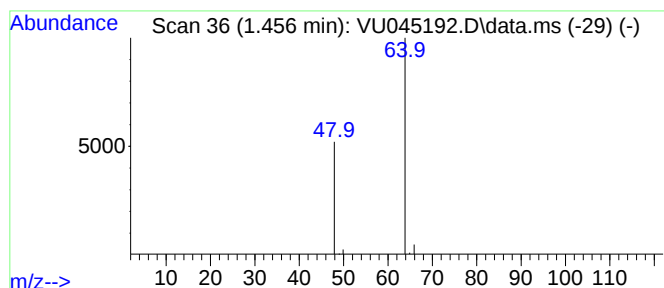
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.456	7.90 ug/L	139385	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW8W9ME

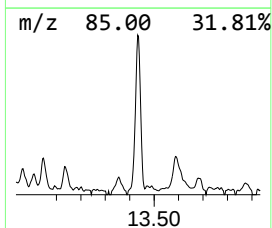
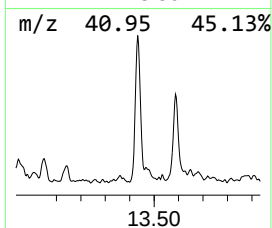
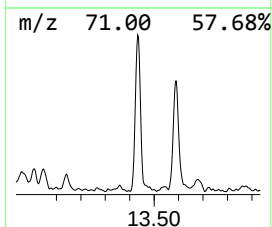
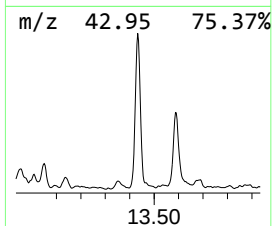
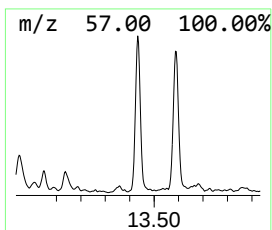
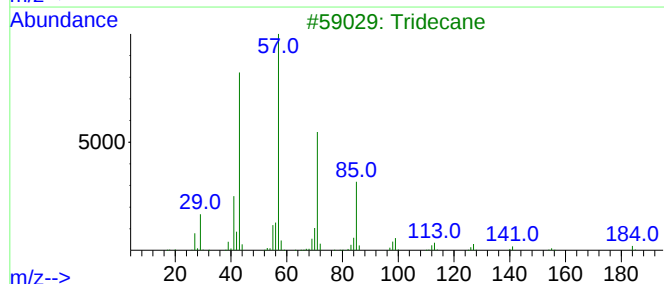
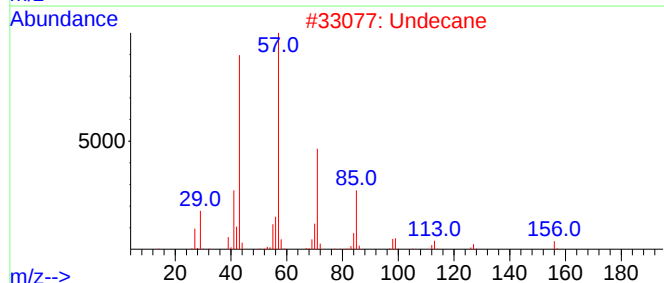
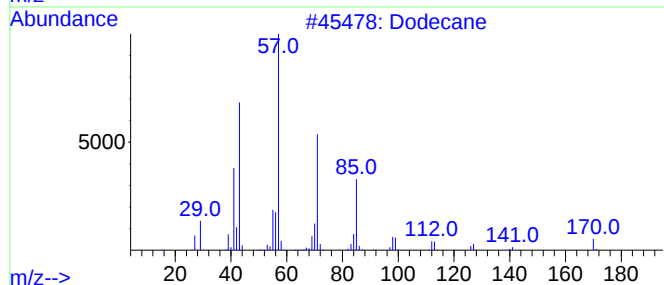
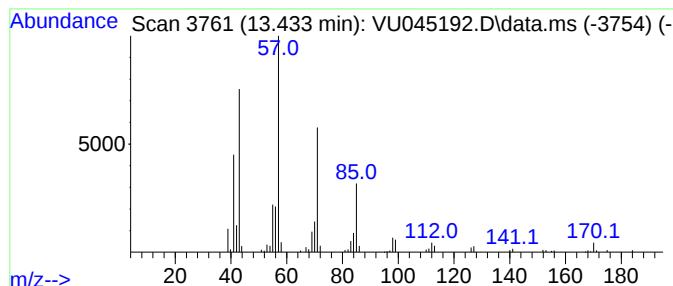
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.433	3.94 ug/L	86087	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	93
2			Undecane	156	C11H24	001120-21-4	90
3			Tridecane	184	C13H28	000629-50-5	87
4			Dodecane	170	C12H26	000112-40-3	87
5			Hexadecane	226	C16H34	000544-76-3	86



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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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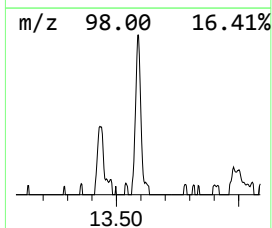
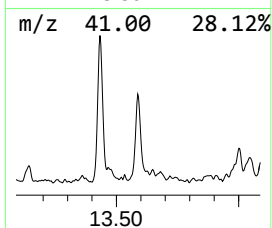
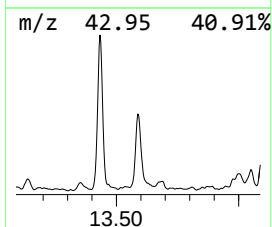
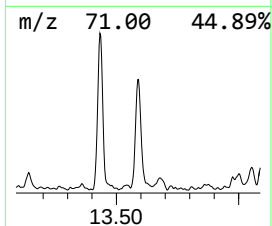
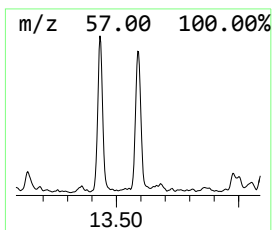
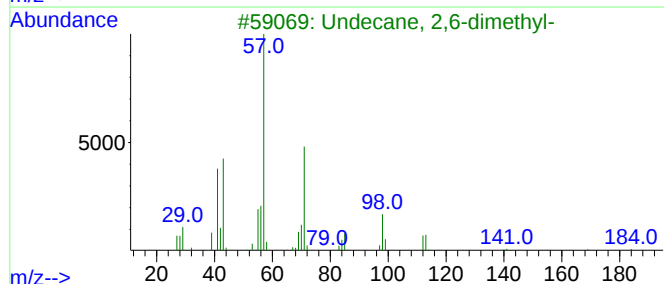
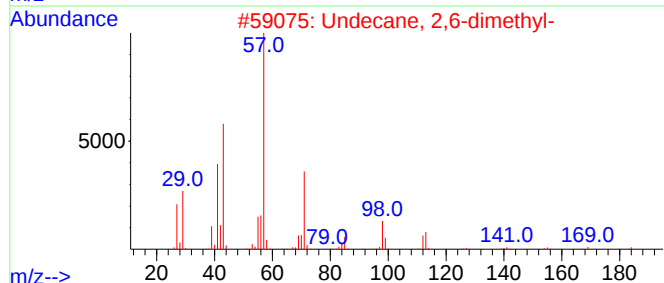
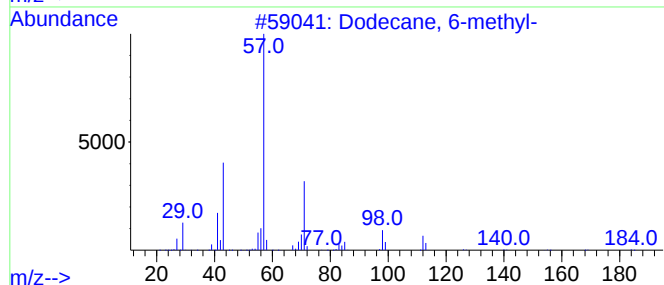
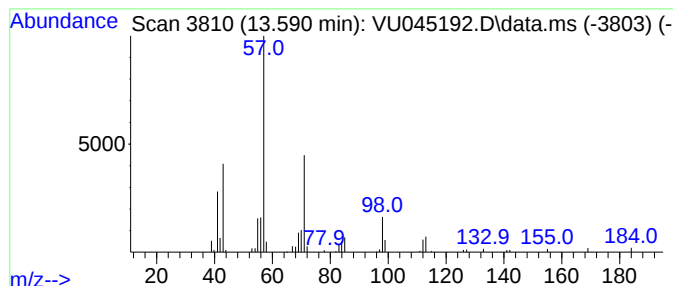
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Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.590	2.57 ug/L	56244	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 6-methyl-	184	C13H28	006044-71-9	91
2			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	90
3			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	90
4			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	87
5			Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100621\
Data File : VU045192.D
Acq On : 06 Oct 2021 17:48
Operator : SY/MD
Sample : M3973-03ME
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW8W9ME

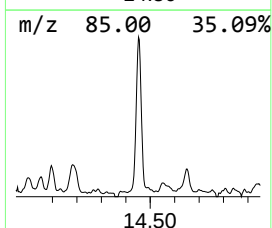
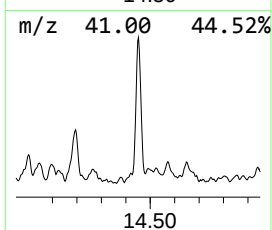
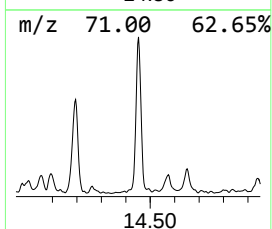
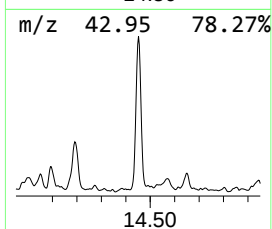
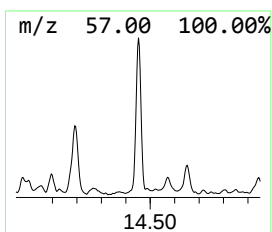
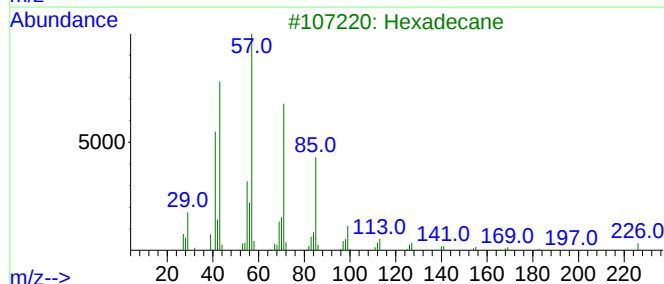
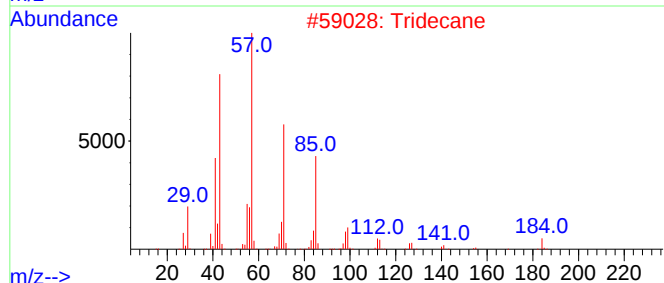
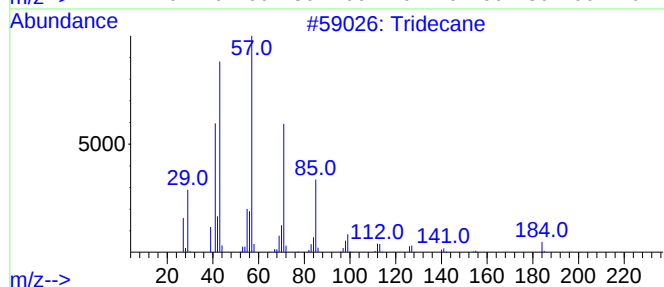
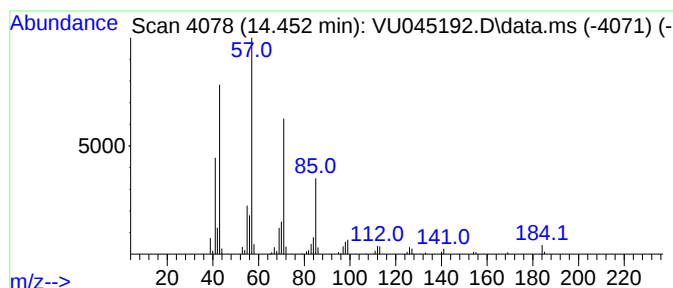
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Quant Title : VOC Analysis

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.452	3.97 ug/L	86698	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	96
2			Tridecane	184	C13H28	000629-50-5	95
3			Hexadecane	226	C16H34	000544-76-3	91
4			Tridecane	184	C13H28	000629-50-5	91
5			Dodecane	170	C12H26	000112-40-3	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100621\
Data File : VU045192.D
Acq On : 06 Oct 2021 17:48
Operator : SY/MD
Sample : M3973-03ME
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW8W9ME

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	1.456	7.9	ug/L	139385	1	6.250	881693	50.0
(DEL) Alkane: S...	13.433	3.9	ug/L	86087	3	11.819	1092580	50.0
(DEL) Alkane: S...	13.590	2.6	ug/L	56244	3	11.819	1092580	50.0
(DEL) Alkane: S...	14.452	4.0	ug/L	86698	3	11.819	1092580	50.0