

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100421\
 Data File : VU045096.D
 Acq On : 04 Oct 2021 15:12
 Operator : SY/MD
 Sample : M3996-04
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F4A16

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: VU045096.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.466	32	39	61	rBV	71367	152241	1.03%	0.557%
2	1.601	75	81	94	rVB	221039	249778	1.68%	0.913%
3	1.897	166	173	191	rVB	139549	200624	1.35%	0.733%
4	1.983	194	200	214	rVB	27865	40023	0.27%	0.146%
5	2.466	341	350	361	rVB	27175	43395	0.29%	0.159%
6	2.565	367	381	400	rBV	298184	491463	3.31%	1.797%
7	2.794	444	452	462	rBV3	1056	1628	0.01%	0.006%
8	2.958	496	503	504	rBV2	301	380	0.00%	0.001%
9	3.019	512	522	525	rBV3	3246	5045	0.03%	0.018%
10	3.138	550	559	564	rBV2	2694	4830	0.03%	0.018%
11	3.189	569	575	589	rVB2	4593	9426	0.06%	0.034%
12	3.366	616	630	650	rVB3	21299	49791	0.34%	0.182%
13	3.572	685	694	699	rVV3	770	1275	0.01%	0.005%
14	3.707	729	736	741	rVB3	454	600	0.00%	0.002%
15	3.839	771	777	785	rBV4	371	551	0.00%	0.002%
16	3.919	795	802	807	rBV3	560	753	0.01%	0.003%
17	3.974	810	819	821	rBV3	1629	1925	0.01%	0.007%
18	4.083	847	853	854	rBV2	612	543	0.00%	0.002%
19	4.096	854	857	860	rVV3	455	312	0.00%	0.001%
20	4.334	923	931	933	rBV4	1856	2247	0.02%	0.008%
21	4.533	982	993	1007	rVB5	3963	9349	0.06%	0.034%
22	4.623	1007	1021	1061	rBV	156828	378864	2.55%	1.385%
23	4.977	1126	1131	1136	rBV2	340	346	0.00%	0.001%
24	5.067	1143	1159	1179	rBV	242426	532168	3.59%	1.945%
25	5.183	1185	1195	1204	rBV2	2194	3911	0.03%	0.014%
26	5.292	1223	1229	1236	rVB2	521	812	0.01%	0.003%
27	5.388	1248	1259	1270	rBV6	2548	5305	0.04%	0.019%
28	5.456	1276	1280	1284	rBV3	651	761	0.01%	0.003%
29	5.729	1342	1365	1376	rBV2	519669	1429024	9.63%	5.224%
30	5.897	1413	1417	1432	rVB9	1893	3338	0.02%	0.012%
31	5.980	1441	1443	1449	rVB4	413	370	0.00%	0.001%
32	6.112	1480	1484	1485	rBV	440	345	0.00%	0.001%
33	6.253	1513	1528	1551	rBV	370438	699699	4.72%	2.558%
34	6.546	1607	1619	1630	rBV6	11775	21830	0.15%	0.080%
35	6.694	1651	1665	1684	rBV	324498	631242	4.25%	2.308%
36	7.044	1765	1774	1777	rBV2	799	1071	0.01%	0.004%

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Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF Filtering: 5
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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
 Title : VOC Analysis

37	7.109	1785	1794	1804	rVB3	1380	2358	0.02%	0.009%
38	7.176	1804	1815	1816	rBV3	1944	2071	0.01%	0.008%
39	7.379	1875	1878	1880	rBV	793	541	0.00%	0.002%
40	7.568	1924	1937	1953	rBV	189861	325162	2.19%	1.189%
41	7.694	1965	1976	1990	rVB9	2194	4976	0.03%	0.018%
42	7.803	2003	2010	2012	rBV2	383	391	0.00%	0.001%
43	7.900	2026	2040	2053	rBV	653344	1123504	7.57%	4.107%
44	7.974	2053	2063	2079	rVB	124208	213897	1.44%	0.782%
45	8.183	2116	2128	2146	rBV	131719	214839	1.45%	0.785%
46	8.475	2213	2219	2228	rBV3	600	927	0.01%	0.003%
47	8.559	2228	2245	2259	rBV	8875453	14835408	100.00%	54.232%
48	8.636	2260	2269	2301	rVB	501303	910363	6.14%	3.328%
49	8.835	2326	2331	2337	rVB2	1011	1063	0.01%	0.004%
50	9.350	2484	2491	2496	rVB4	624	769	0.01%	0.003%
51	9.420	2499	2513	2530	rBV	532783	858408	5.79%	3.138%
52	9.575	2549	2561	2576	rBV	69582	111279	0.75%	0.407%
53	9.697	2587	2599	2612	rBV	64510	105382	0.71%	0.385%
54	10.102	2714	2725	2739	rBV	49733	80699	0.54%	0.295%
55	10.420	2821	2824	2828	rBV2	278	313	0.00%	0.001%
56	10.488	2836	2845	2851	rBV2	2575	3324	0.02%	0.012%
57	10.674	2894	2903	2913	rVV2	5188	7905	0.05%	0.029%
58	10.761	2916	2930	2953	rVV	474429	759099	5.12%	2.775%
59	10.871	2955	2964	2966	rVV3	893	1325	0.01%	0.005%
60	10.909	2966	2976	2990	rVB2	12135	20095	0.14%	0.073%
61	11.002	2995	3005	3009	rBV	16109	24499	0.17%	0.090%
62	11.092	3024	3033	3050	rBV2	8306	13052	0.09%	0.048%
63	11.205	3064	3068	3073	rBV4	472	557	0.00%	0.002%
64	11.295	3085	3096	3109	rVB2	10844	16073	0.11%	0.059%
65	11.469	3139	3150	3168	rVB	52479	84769	0.57%	0.310%
66	11.581	3179	3185	3192	rBV3	1045	1415	0.01%	0.005%
67	11.700	3214	3222	3231	rVB4	2372	3374	0.02%	0.012%
68	11.742	3231	3235	3238	rBV2	403	410	0.00%	0.001%
69	11.816	3245	3258	3275	rBV	553305	871135	5.87%	3.185%
70	11.899	3275	3284	3293	rVB2	10095	14720	0.10%	0.054%
71	11.977	3303	3308	3316	rVB3	4020	5307	0.04%	0.019%
72	12.099	3332	3346	3360	rBV3	21526	37403	0.25%	0.137%
73	12.195	3360	3376	3394	rVB	647288	1042408	7.03%	3.811%
74	12.301	3406	3409	3410	rBV2	506	354	0.00%	0.001%
75	12.385	3428	3435	3438	rBV5	909	1162	0.01%	0.004%
76	12.469	3452	3461	3466	rBV4	2473	3467	0.02%	0.013%

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 Title : VOC Analysis

77	12.575	3484	3494	3501	rBV2	6624	9899	0.07%	0.036%
78	12.684	3524	3528	3536	rVB3	3566	4371	0.03%	0.016%
79	12.803	3560	3565	3568	rBV4	845	872	0.01%	0.003%
80	12.977	3610	3619	3627	rBV2	3815	5517	0.04%	0.020%
81	13.028	3627	3635	3646	rVB2	4773	7513	0.05%	0.027%
82	13.144	3666	3671	3676	rBV4	934	1098	0.01%	0.004%
83	13.295	3710	3718	3731	rVB	4659	6238	0.04%	0.023%
84	13.411	3745	3754	3757	rBV3	383	583	0.00%	0.002%
85	13.456	3760	3768	3779	rVB3	10373	16318	0.11%	0.060%
86	13.523	3784	3789	3796	rBV4	867	1125	0.01%	0.004%
87	13.626	3817	3821	3822	rBV3	1546	1073	0.01%	0.004%
88	13.832	3882	3885	3888	rBV3	693	562	0.00%	0.002%
89	14.089	3953	3965	3981	rBV	138210	226917	1.53%	0.830%
90	14.211	3993	4003	4015	rVB	21168	33318	0.22%	0.122%
91	14.488	4085	4089	4095	rVB4	1058	1177	0.01%	0.004%
92	14.809	4184	4189	4195	rBV4	861	1258	0.01%	0.005%
93	14.880	4205	4211	4225	rVB3	2879	4574	0.03%	0.017%
94	15.173	4293	4302	4308	rBV2	7272	10735	0.07%	0.039%
95	15.227	4308	4319	4337	rVB	95640	168167	1.13%	0.615%
96	15.340	4348	4354	4364	rVB3	5841	9192	0.06%	0.034%
97	15.414	4366	4377	4395	rVB2	86558	150706	1.02%	0.551%
98	16.115	4592	4595	4597	rBV2	653	488	0.00%	0.002%
99	16.266	4636	4642	4651	rBV5	3260	5436	0.04%	0.020%
100	16.411	4681	4687	4694	rBV3	6418	8763	0.06%	0.032%

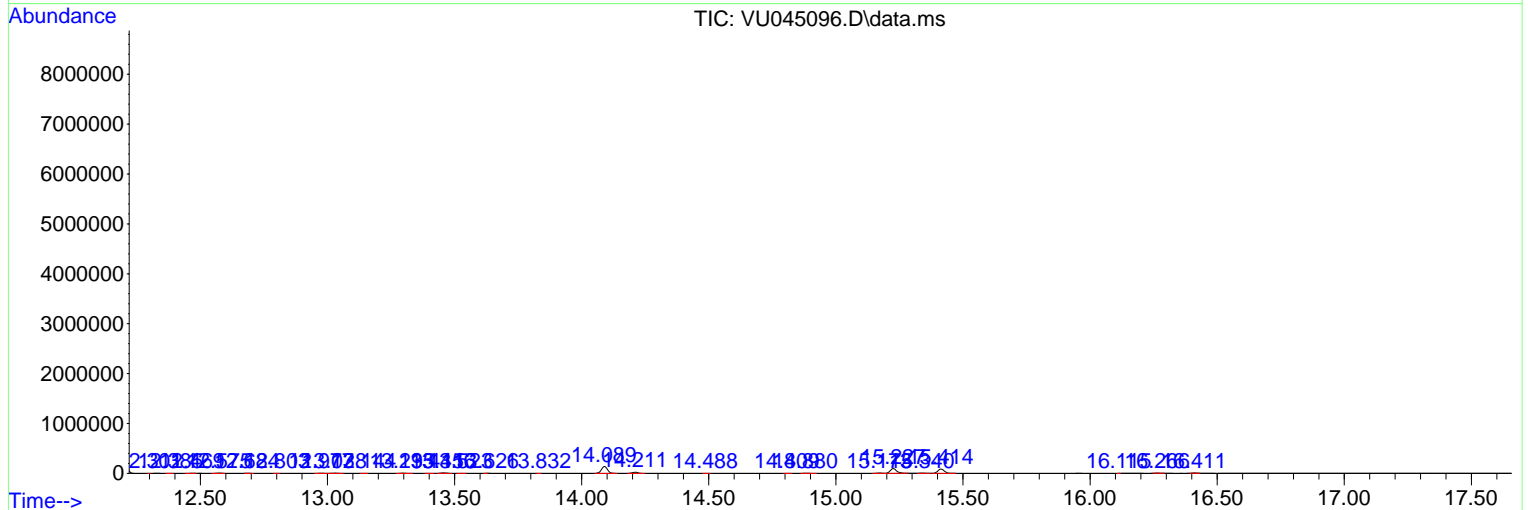
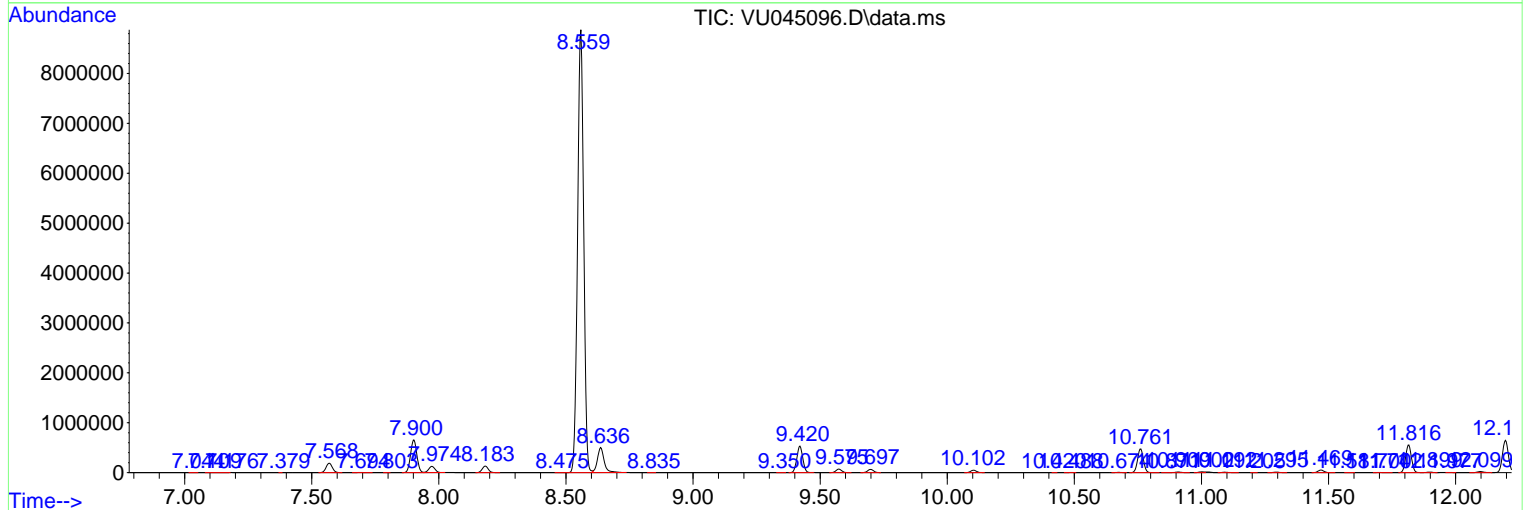
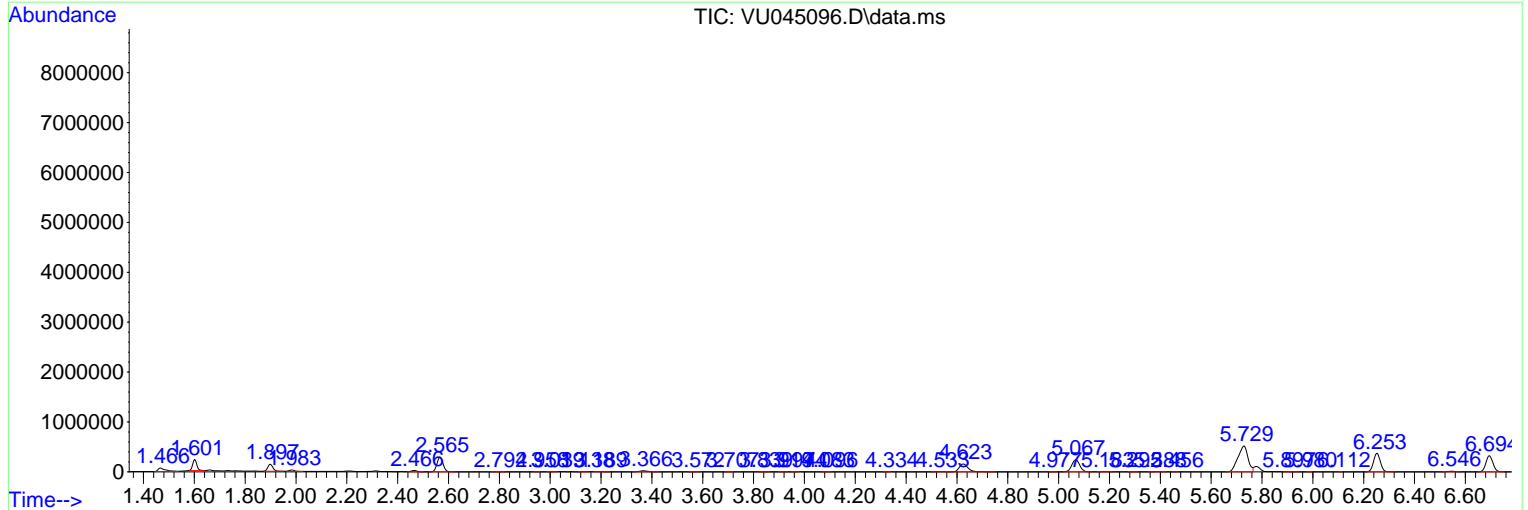
Sum of corrected areas: 27355368

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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



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 Operator : SY/MD
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 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampled :
 F4A16

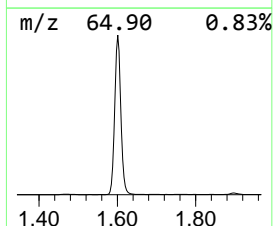
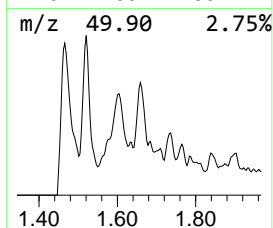
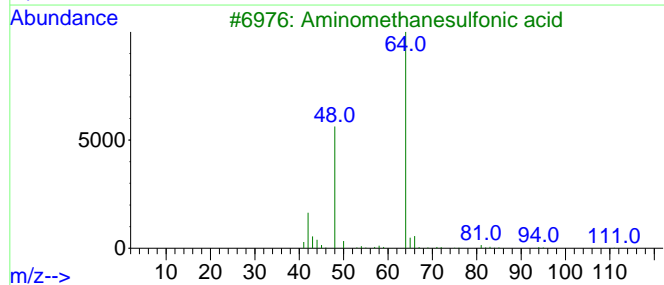
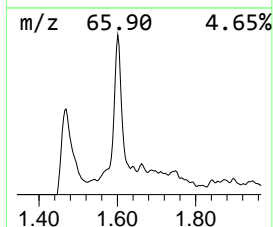
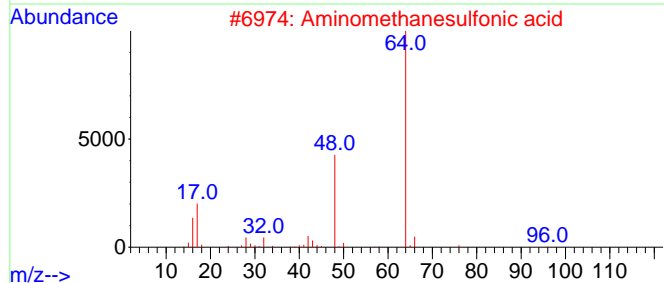
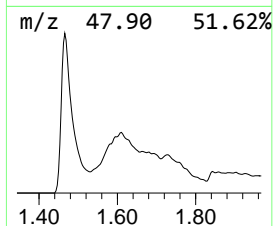
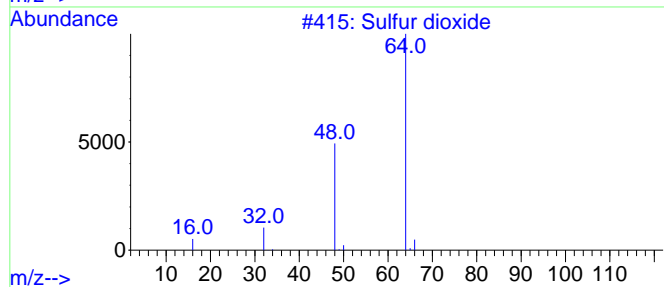
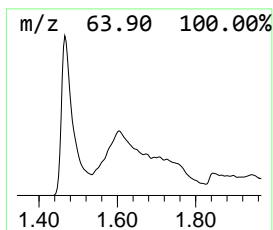
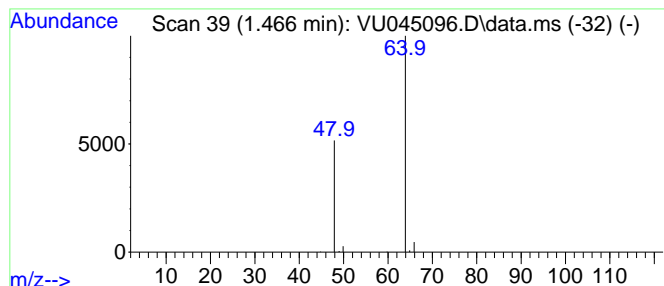
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
 Quant Title : VOC Analysis

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

 Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.466	10.88 ug/L	152241	1,4-Difluorobenzene	6.253

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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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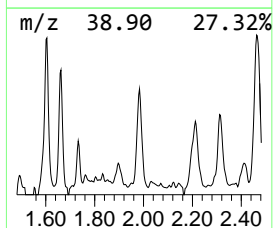
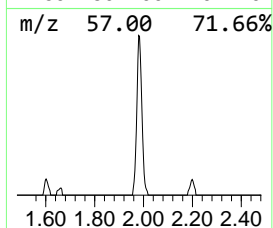
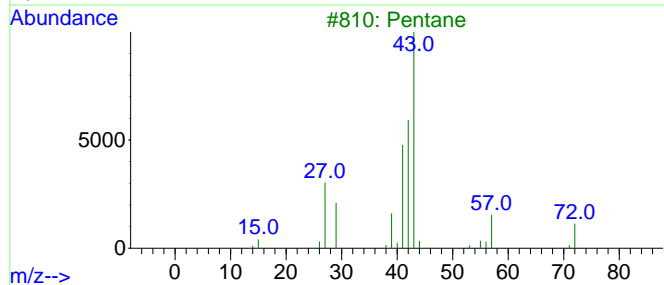
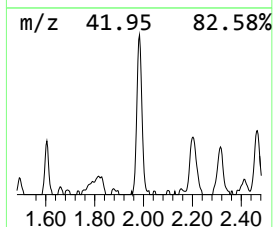
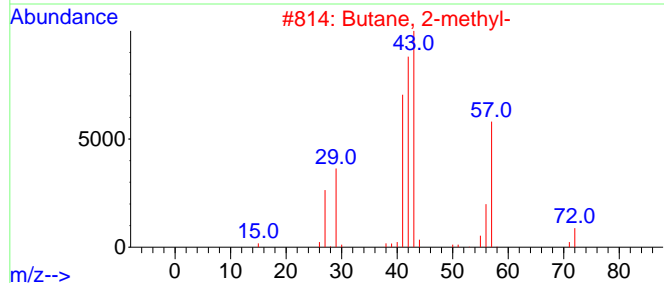
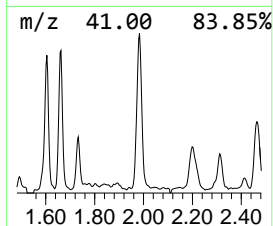
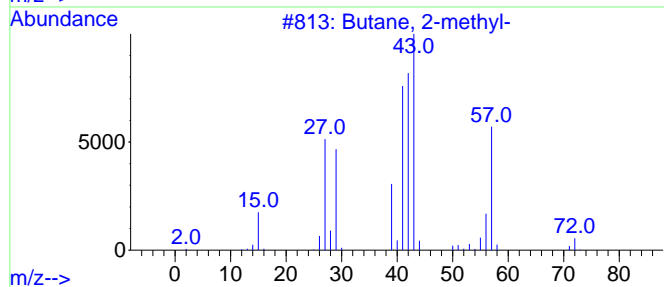
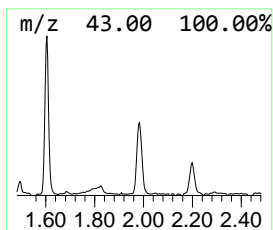
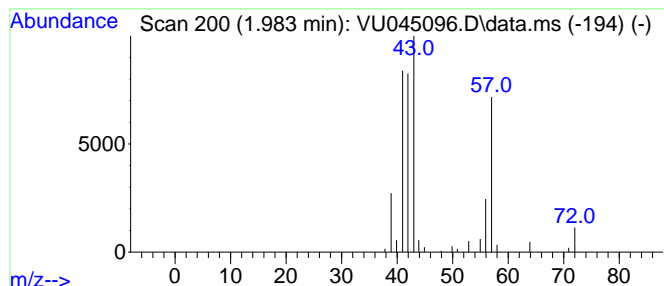
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
 Quant Title : VOC Analysis

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

 Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.983	2.86 ug/L	40023	1,4-Difluorobenzene	6.253

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methyl-	72	C5H12	000078-78-4	87
2		Butane, 2-methyl-	72	C5H12	000078-78-4	87
3		Pentane	72	C5H12	000109-66-0	59
4		Pentane	72	C5H12	000109-66-0	45
5		3-Buten-1-ol	72	C4H8O	000627-27-0	38



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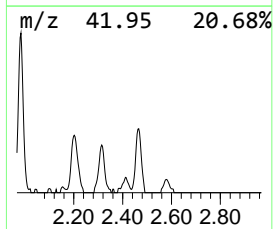
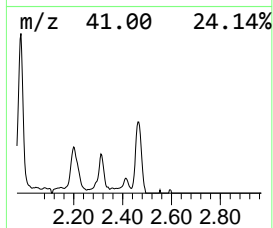
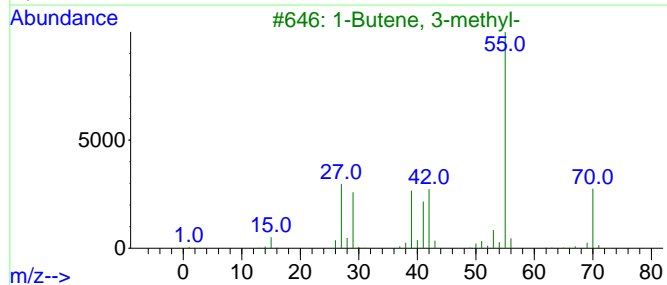
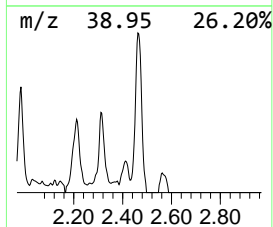
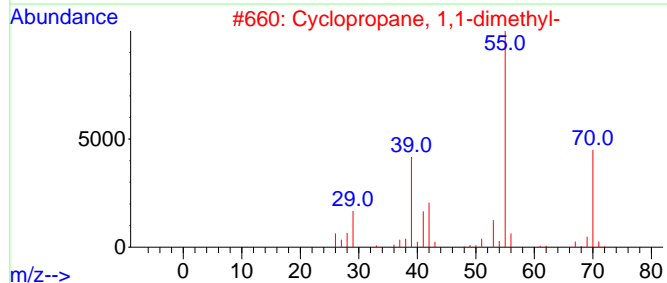
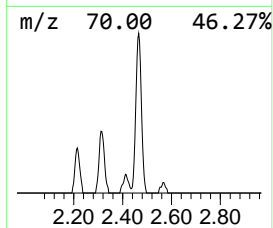
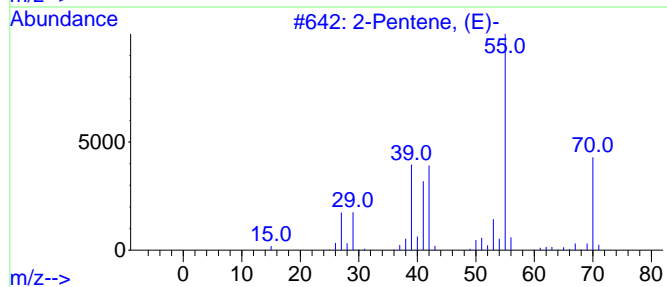
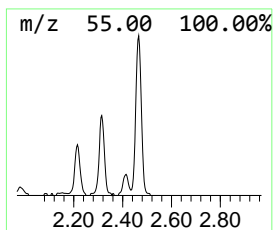
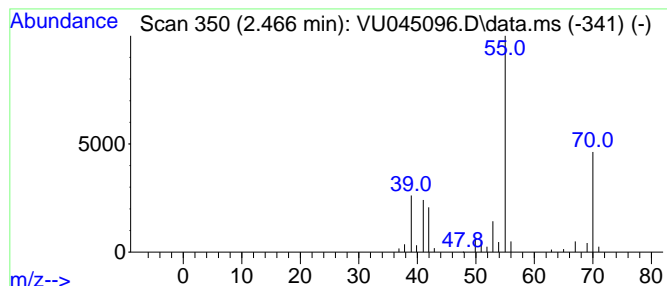
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
 Quant Title : VOC Analysis

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

 Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.466	3.10 ug/L	43395	1,4-Difluorobenzene	6.253

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentene, (E)-	70	C5H10	000646-04-8	86
2		Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80
3		1-Butene, 3-methyl-	70	C5H10	000563-45-1	78
4		2-Methyl-1-butene	70	C5H10	000563-46-2	72
5		1-Butene, 3-methyl-	70	C5H10	000563-45-1	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100421\
 Data File : VU045096.D
 Acq On : 04 Oct 2021 15:12
 Operator : SY/MD
 Sample : M3996-04
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F4A16

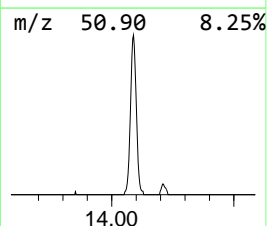
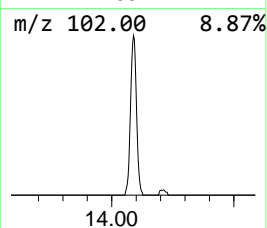
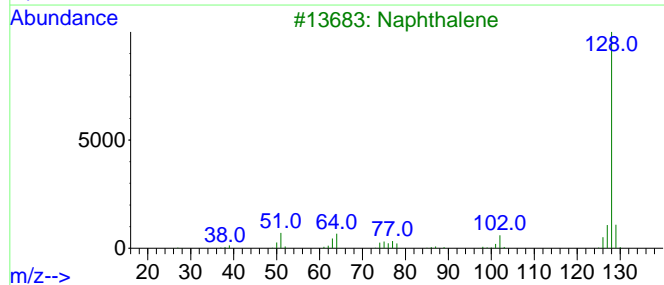
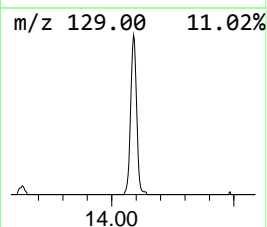
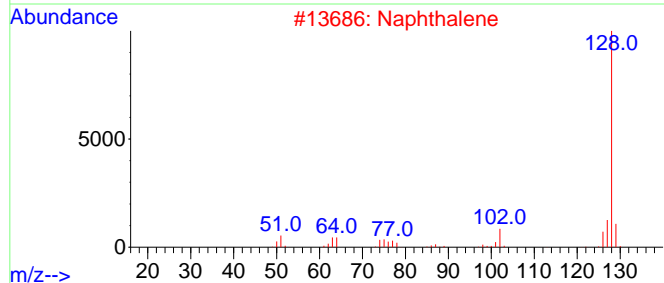
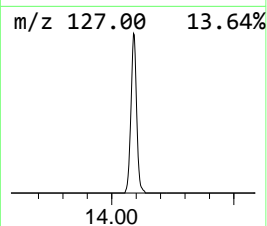
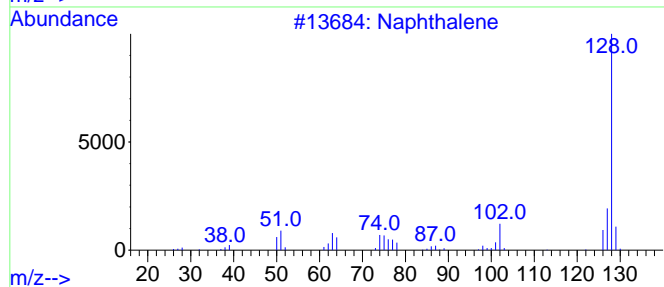
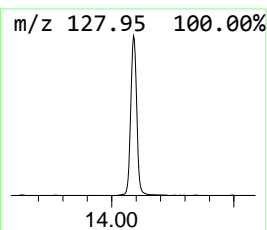
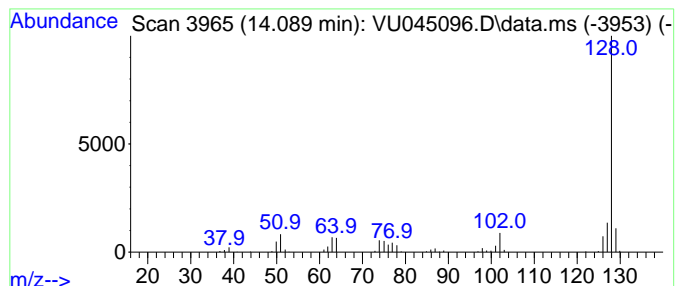
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 Quant Title : VOC Analysis

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

 Peak Number 5 Azulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.089	13.02 ug/L	226917	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	97
2			Naphthalene	128	C10H8	000091-20-3	95
3			Naphthalene	128	C10H8	000091-20-3	94
4			Naphthalene	128	C10H8	000091-20-3	93
5			Azulene	128	C10H8	000275-51-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100421\
 Data File : VU045096.D
 Acq On : 04 Oct 2021 15:12
 Operator : SY/MD
 Sample : M3996-04
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
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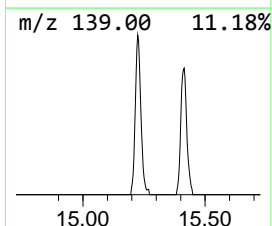
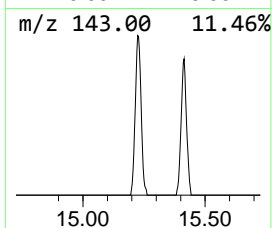
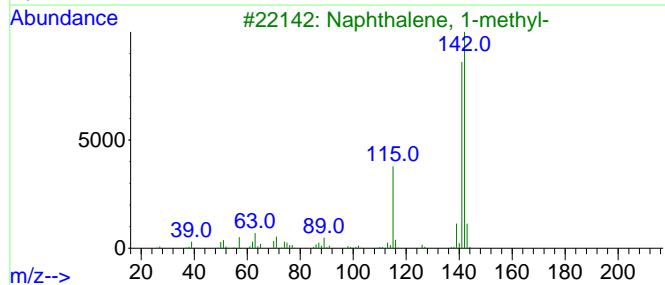
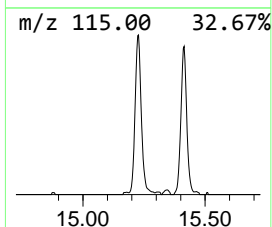
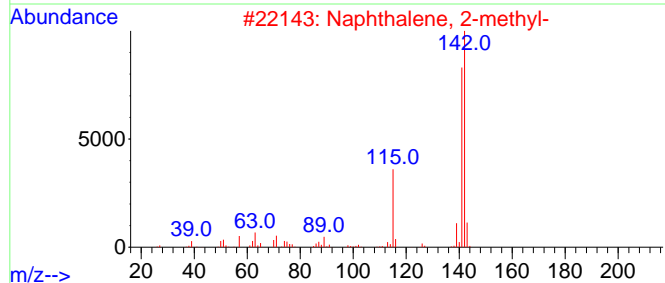
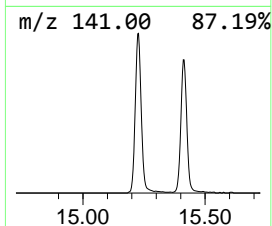
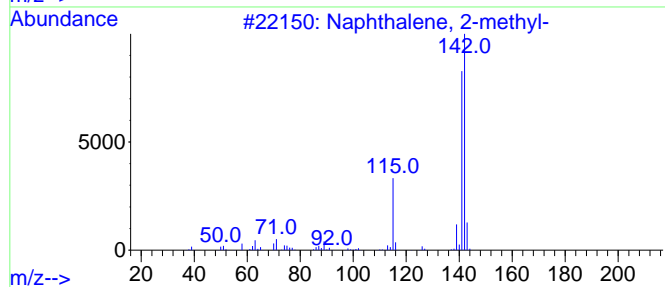
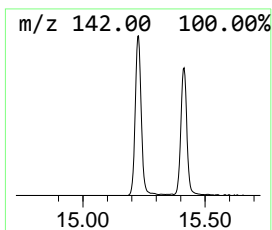
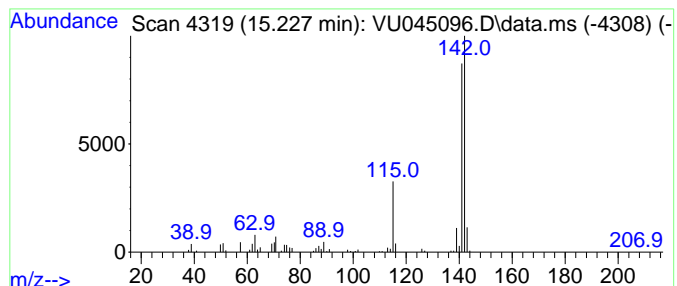
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 Quant Title : VOC Analysis

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

 Peak Number 6 Naphthalene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.227	9.65 ug/L	168167	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
4			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	95
5			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100421\
 Data File : VU045096.D
 Acq On : 04 Oct 2021 15:12
 Operator : SY/MD
 Sample : M3996-04
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F4A16

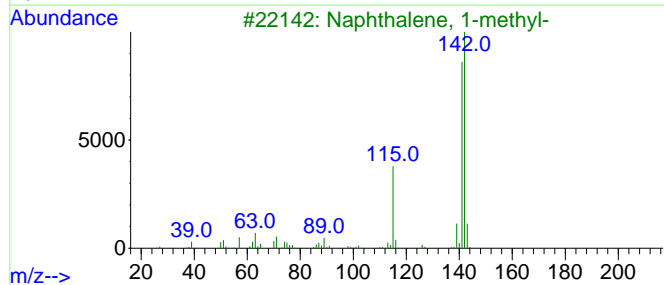
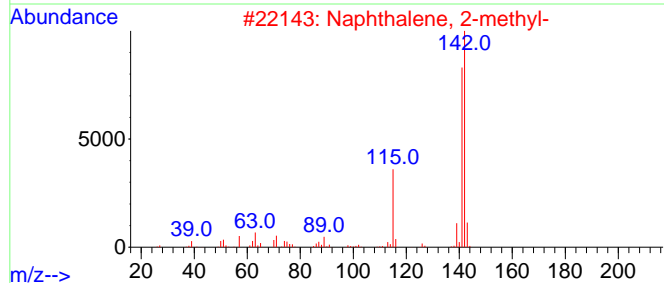
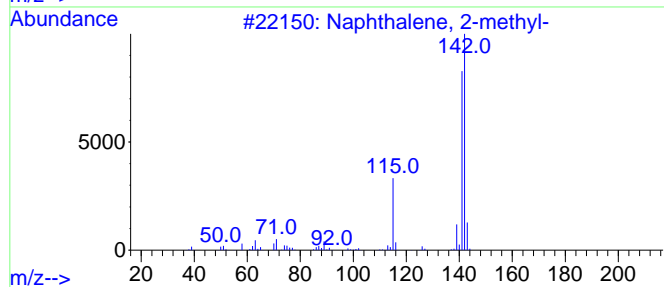
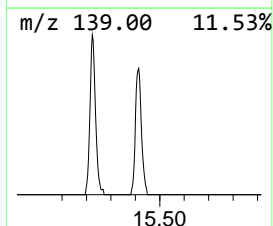
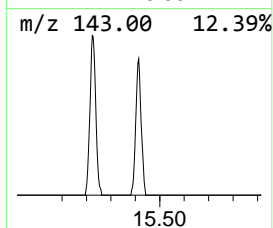
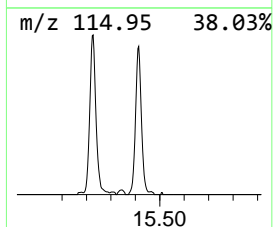
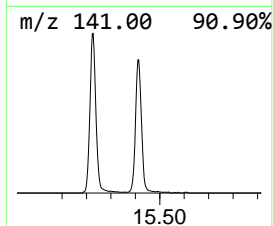
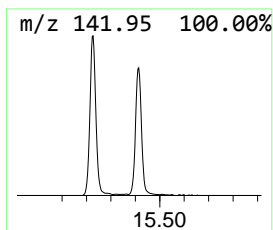
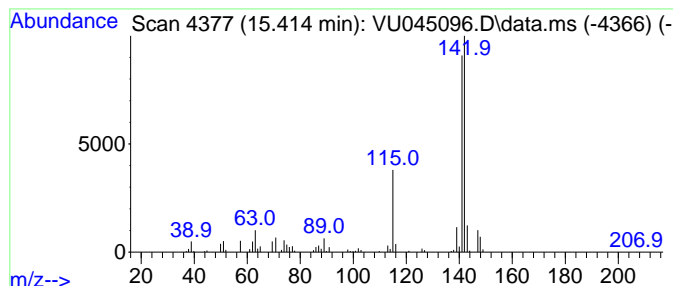
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 Quant Title : VOC Analysis

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

 Peak Number 7 Naphthalene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.414	8.65 ug/L	150706	1,4-Dichlorobenzene-d4	11.816

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100421\
Data File : VU045096.D
Acq On : 04 Oct 2021 15:12
Operator : SY/MD
Sample : M3996-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F4A16

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	1.466	10.9	ug/L	152241	1	6.253	699699	50.0
(DEL) Alkane: S...	1.983	2.9	ug/L	40023	1	6.253	699699	50.0
(DEL) Alkane: S...	2.466	3.1	ug/L	43395	1	6.253	699699	50.0
Azulene	14.089	13.0	ug/L	226917	3	11.816	871135	50.0
Naphthalene, 2-...	15.227	9.7	ug/L	168167	3	11.816	871135	50.0
Naphthalene, 1-...	15.414	8.7	ug/L	150706	3	11.816	871135	50.0