

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012723\
 Data File : VU052836.D
 Acq On : 27 Jan 2023 11:07
 Operator : JC/MD
 Sample : 01316-04
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A44G8

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\SFAMULM012623WMA.M
 Title : VOC Analysis

Signal : TIC: VU052836.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.389	8	15	25	rVB	275362	292785	29.77%	3.022%
2	1.434	26	29	36	rVB2	7023	6825	0.69%	0.070%
3	1.601	69	81	91	rBV	107232	142493	14.49%	1.471%
4	1.729	114	121	132	rVB	42438	53389	5.43%	0.551%
5	1.790	133	140	148	rBV	12650	16156	1.64%	0.167%
6	1.909	170	177	193	rVB	86745	119739	12.18%	1.236%
7	2.080	224	230	241	rVB	9915	12978	1.32%	0.134%
8	2.372	311	321	336	rVB	178921	266316	27.08%	2.749%
9	2.565	368	381	394	rBV	200072	324876	33.03%	3.354%
10	2.636	395	403	421	rVB	23000	40443	4.11%	0.417%
11	2.916	487	490	495	rBV2	242	293	0.03%	0.003%
12	2.977	506	509	512	rBV2	362	240	0.02%	0.002%
13	3.186	555	574	611	rBV3	208739	744466	75.70%	7.685%
14	3.565	686	692	694	rBV2	982	987	0.10%	0.010%
15	3.700	730	734	735	rBV	186	131	0.01%	0.001%
16	3.848	773	780	782	rBV	542	568	0.06%	0.006%
17	3.864	782	785	787	rBV2	558	385	0.04%	0.004%
18	3.990	808	824	843	rVB3	13764	36415	3.70%	0.376%
19	4.128	857	867	870	rBV4	937	1620	0.16%	0.017%
20	4.366	938	941	944	rBB	348	249	0.03%	0.003%
21	4.405	950	953	955	rBV	248	163	0.02%	0.002%
22	4.443	961	965	966	rBV	256	173	0.02%	0.002%
23	4.617	1000	1019	1061	rBV2	246219	704506	71.64%	7.273%
24	5.057	1141	1156	1177	rBV	192198	422928	43.00%	4.366%
25	5.376	1248	1255	1256	rBV3	2731	2341	0.24%	0.024%
26	5.456	1279	1280	1281	rBV3	341	130	0.01%	0.001%
27	5.488	1287	1290	1294	rVB2	247	176	0.02%	0.002%
28	5.540	1303	1306	1312	rVB2	418	493	0.05%	0.005%
29	5.607	1324	1327	1328	rBV2	260	163	0.02%	0.002%
30	5.720	1341	1362	1374	rBV2	351883	983466	100.00%	10.152%
31	5.935	1421	1429	1434	rBV2	5585	10410	1.06%	0.107%
32	6.134	1485	1491	1497	rBV4	901	1381	0.14%	0.014%
33	6.244	1510	1525	1555	rBV	206759	391540	39.81%	4.042%
34	6.379	1564	1567	1568	rBV	256	137	0.01%	0.001%
35	6.507	1596	1607	1611	rBV4	4690	8958	0.91%	0.092%
36	6.639	1645	1648	1649	rBV	377	211	0.02%	0.002%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM012623WMA.M
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37	6.684	1649	1662	1678	rBV2	218219	424721	43.19%	4.384%
38	6.977	1739	1753	1782	rBV	200327	459620	46.73%	4.745%
39	7.115	1791	1796	1805	rBV5	1875	2873	0.29%	0.030%
40	7.224	1828	1830	1833	rBV5	279	154	0.02%	0.002%
41	7.256	1837	1840	1842	rVB2	367	232	0.02%	0.002%
42	7.382	1875	1879	1882	rBV2	348	197	0.02%	0.002%
43	7.427	1890	1893	1895	rBV2	439	276	0.03%	0.003%
44	7.482	1900	1910	1923	rVB6	3147	6726	0.68%	0.069%
45	7.562	1923	1935	1950	rBV	124706	217289	22.09%	2.243%
46	7.697	1965	1977	1983	rBV8	2843	5142	0.52%	0.053%
47	7.793	2003	2007	2014	rVB2	196	253	0.03%	0.003%
48	7.822	2014	2016	2017	rBV2	271	141	0.01%	0.001%
49	7.893	2025	2038	2054	rBV	451864	775620	78.87%	8.007%
50	8.096	2092	2101	2102	rBV2	871	1081	0.11%	0.011%
51	8.176	2114	2126	2143	rVB	87529	145228	14.77%	1.499%
52	8.240	2143	2146	2147	rBV	364	204	0.02%	0.002%
53	8.308	2160	2167	2174	rBV5	3962	6069	0.62%	0.063%
54	8.446	2206	2210	2212	rBV2	438	416	0.04%	0.004%
55	8.482	2212	2221	2233	rVV2	8760	16308	1.66%	0.168%
56	8.629	2254	2267	2300	rBV2	249043	476844	48.49%	4.922%
57	8.822	2324	2327	2328	rBV	307	160	0.02%	0.002%
58	8.922	2355	2358	2360	rBV	407	323	0.03%	0.003%
59	9.070	2400	2404	2406	rBV2	203	185	0.02%	0.002%
60	9.234	2452	2455	2456	rBV2	260	167	0.02%	0.002%
61	9.266	2459	2465	2477	rVB4	2661	4384	0.45%	0.045%
62	9.334	2478	2486	2497	rVV8	4098	7267	0.74%	0.075%
63	9.414	2499	2511	2540	rVB2	291616	572995	58.26%	5.915%
64	9.594	2553	2567	2577	rBV2	12147	21263	2.16%	0.219%
65	9.684	2585	2595	2608	rVB4	18307	32255	3.28%	0.333%
66	9.755	2608	2617	2624	rBV4	2903	4322	0.44%	0.045%
67	9.806	2628	2633	2637	rBV	649	647	0.07%	0.007%
68	9.822	2637	2638	2644	rVB	443	301	0.03%	0.003%
69	10.054	2704	2710	2718	rBV6	1233	1655	0.17%	0.017%
70	10.131	2731	2734	2736	rBV	220	147	0.01%	0.002%
71	10.186	2744	2751	2755	rBV2	334	556	0.06%	0.006%
72	10.298	2782	2786	2788	rBV	291	236	0.02%	0.002%
73	10.385	2811	2813	2814	rBV	369	200	0.02%	0.002%
74	10.481	2832	2843	2856	rVB	40188	61986	6.30%	0.640%
75	10.636	2887	2891	2899	rVB5	2278	2442	0.25%	0.025%
76	10.703	2904	2912	2915	rBV5	3262	4132	0.42%	0.043%

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77	10.752	2916	2927	2955	rVB	328310	524974	53.38%	5.419%
78	10.896	2962	2972	2987	rVB6	8235	16543	1.68%	0.171%
79	10.951	2987	2989	2991	rBV2	345	216	0.02%	0.002%
80	10.986	2998	3000	3003	rVB	399	214	0.02%	0.002%
81	11.128	3040	3044	3055	rBV5	1325	1522	0.15%	0.016%
82	11.227	3068	3075	3084	rBV5	2075	2690	0.27%	0.028%
83	11.520	3160	3166	3168	rBV3	455	513	0.05%	0.005%
84	11.552	3169	3176	3185	rVB3	3080	4325	0.44%	0.045%
85	11.607	3187	3193	3194	rBV3	807	646	0.07%	0.007%
86	11.713	3221	3226	3227	rBV2	566	406	0.04%	0.004%
87	11.806	3243	3255	3275	rBV	304438	522207	53.10%	5.391%
88	12.057	3325	3333	3336	rBV4	8494	11943	1.21%	0.123%
89	12.189	3362	3374	3393	rVB	435486	730570	74.29%	7.542%
90	12.414	3439	3444	3445	rBV4	906	858	0.09%	0.009%
91	12.568	3486	3492	3500	rVB	5233	6732	0.68%	0.069%
92	12.845	3576	3578	3579	rBV2	513	184	0.02%	0.002%
93	12.970	3609	3617	3627	rBV8	3163	5719	0.58%	0.059%
94	13.198	3686	3688	3691	rBV	586	405	0.04%	0.004%
95	13.224	3691	3696	3704	rVB6	3417	4610	0.47%	0.048%
96	13.359	3736	3738	3742	rBV3	433	338	0.03%	0.003%
97	13.443	3756	3764	3775	rVB5	4319	6818	0.69%	0.070%
98	13.674	3833	3836	3837	rBV	1193	542	0.06%	0.006%
99	14.021	3942	3944	3947	rBV	489	202	0.02%	0.002%
100	14.677	4145	4148	4149	rBV2	781	419	0.04%	0.004%

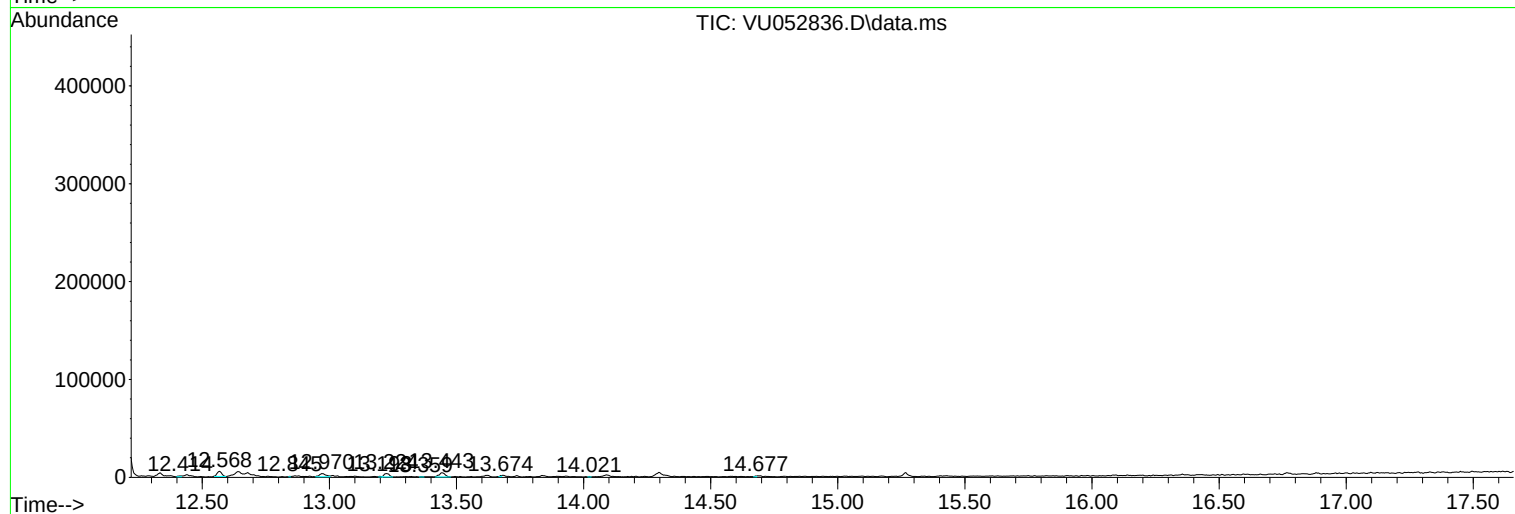
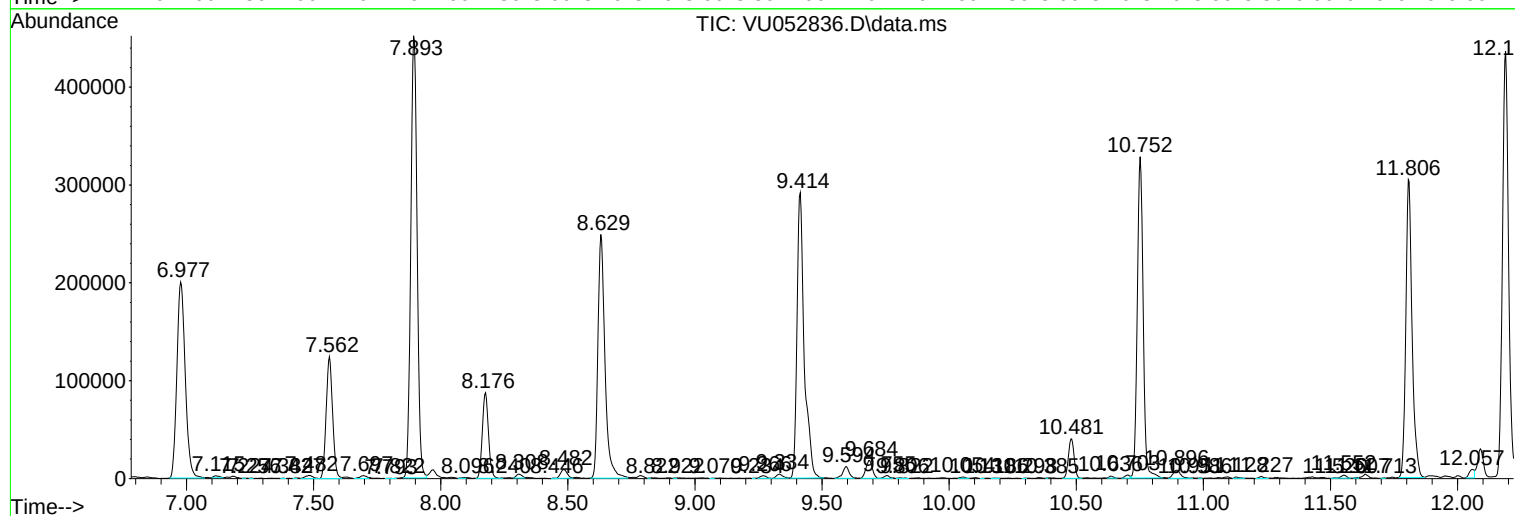
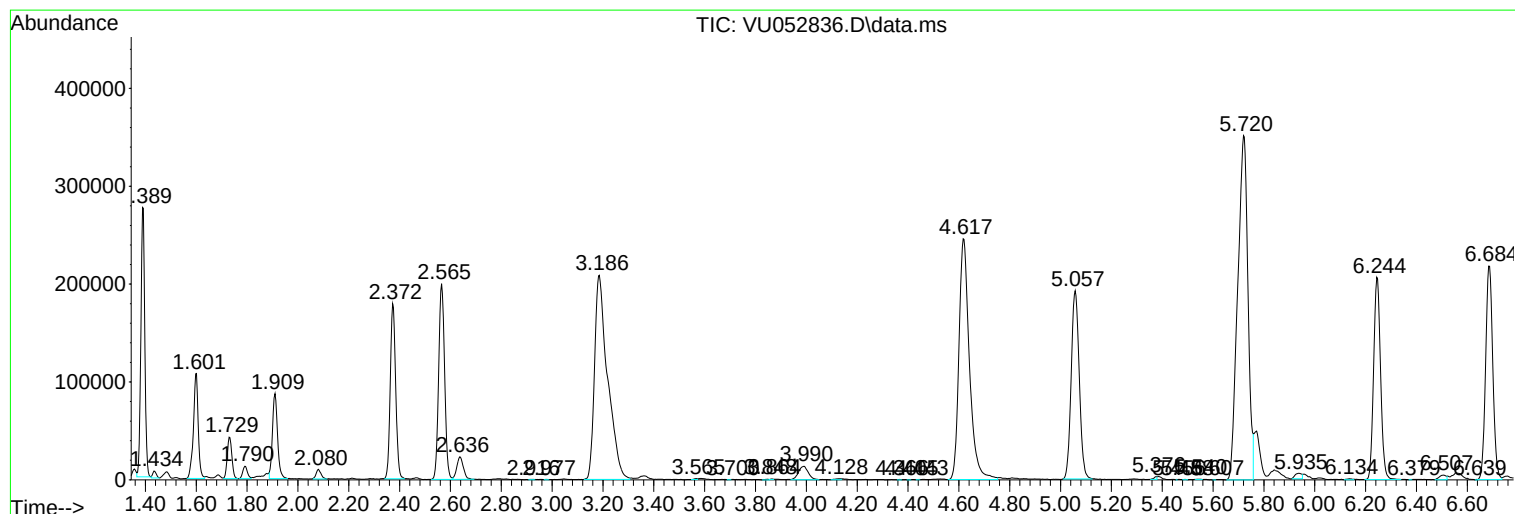
Sum of corrected areas: 9687143

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM012623WMA.M
Quant Title : VOC Analysis

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



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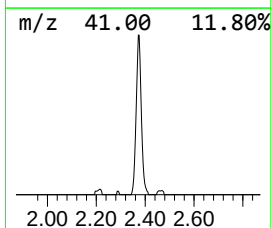
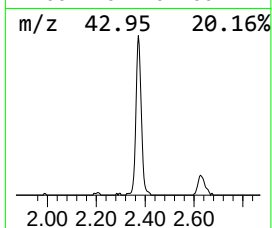
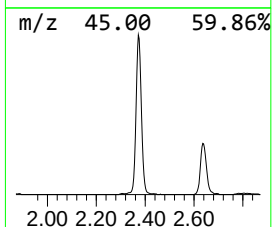
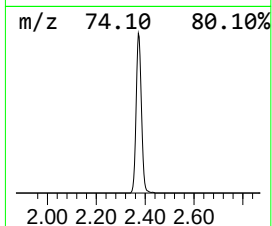
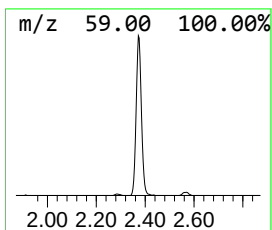
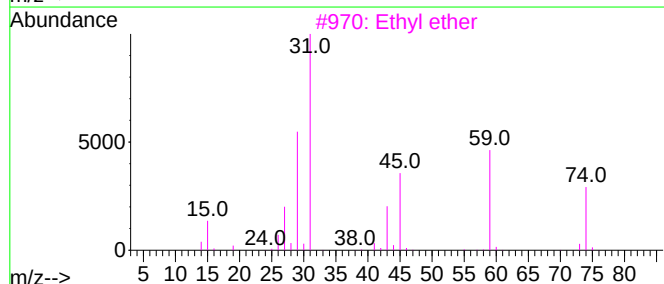
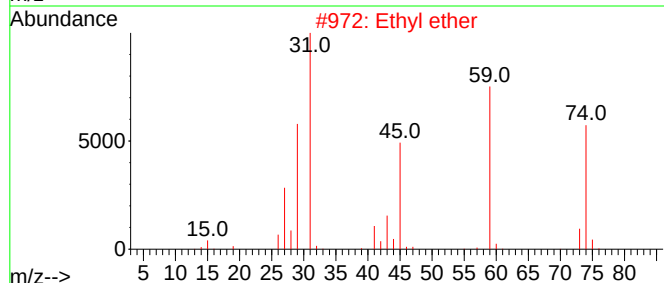
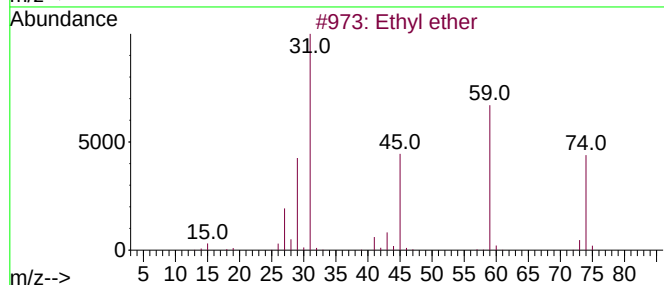
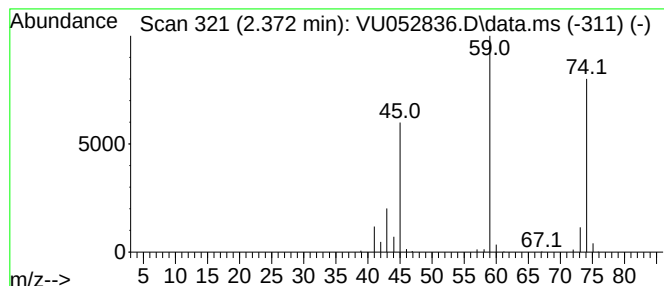
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM012623WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Ethyl ether Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.372	34.01 ug/L	266316	1,4-Difluorobenzene	6.244

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl ether			74	C4H10O	000060-29-7	90
2	Ethyl ether			74	C4H10O	000060-29-7	90
3	Ethyl ether			74	C4H10O	000060-29-7	83
4	Ethyl ether			74	C4H10O	000060-29-7	80
5	Ethane, 1,2-diethoxy-			118	C6H14O2	000629-14-1	64



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Instrument :
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ClientSampleId :
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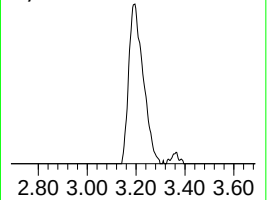
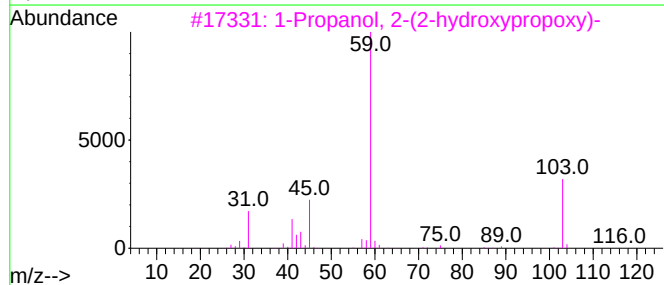
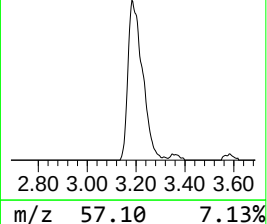
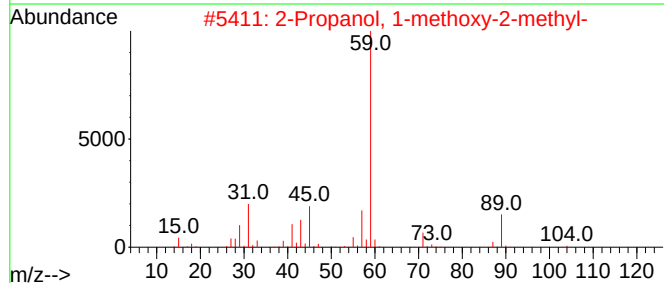
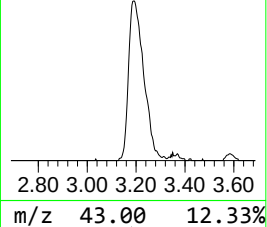
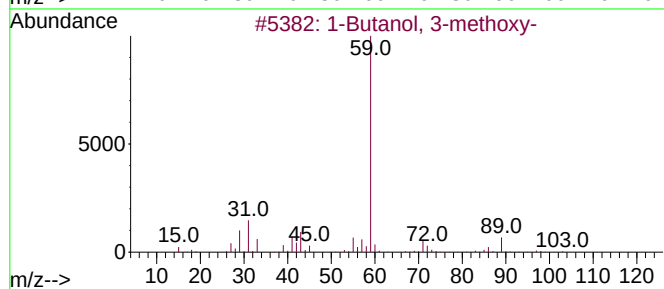
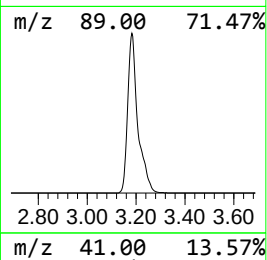
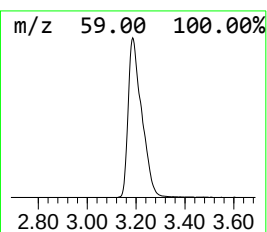
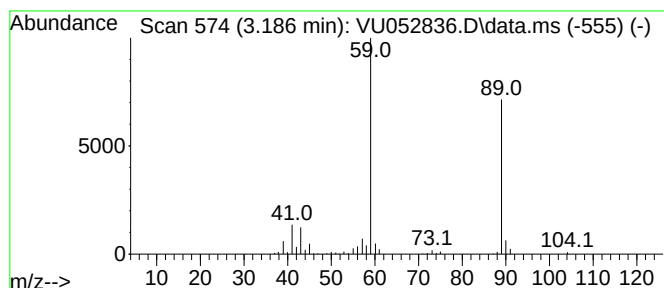
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM012623WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 1-Butanol, 3-methoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.186	95.07 ug/L	744466	1,4-Difluorobenzene	6.244

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol, 3-methoxy-			104	C5H12O2	002517-43-3	56
2	2-Propanol, 1-methoxy-2-methyl-			104	C5H12O2	003587-64-2	56
3	1-Propanol, 2-(2-hydroxypropoxy)-			134	C6H14O3	000106-62-7	47
4	Propane, 1,2-dimethoxy-			104	C5H12O2	007778-85-0	43
5	Methanol, TMS derivative			104	C4H12OSi	001825-61-2	43



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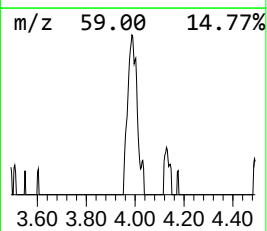
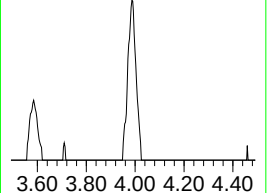
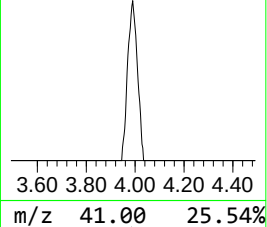
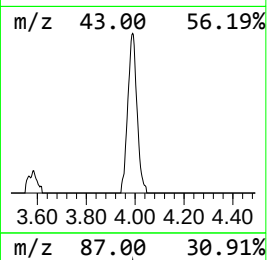
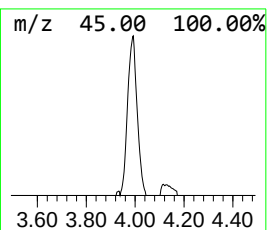
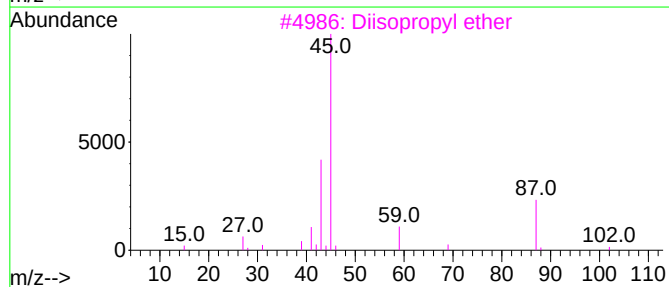
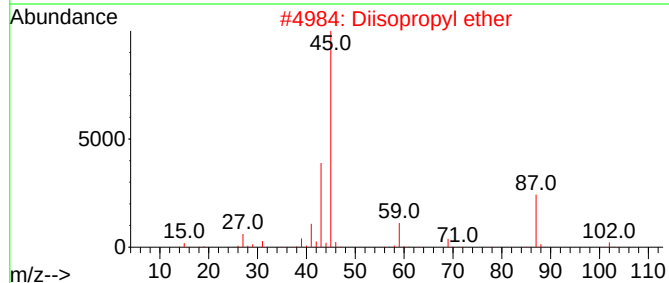
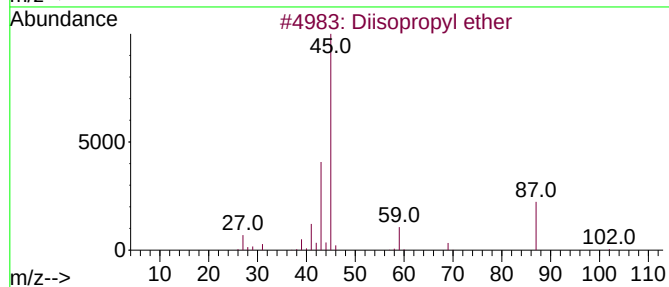
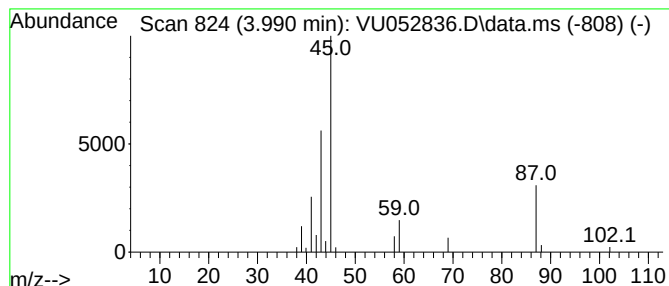
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM012623WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Diisopropyl ether Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.990	4.65 ug/L	36415	1,4-Difluorobenzene	6.244

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diisopropyl ether	102	C6H14O	000108-20-3	78
2			Diisopropyl ether	102	C6H14O	000108-20-3	78
3			Diisopropyl ether	102	C6H14O	000108-20-3	78
4			Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	72
5			1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012723\
Data File : VU052836.D
Acq On : 27 Jan 2023 11:07
Operator : JC/MD
Sample : 01316-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A44G8

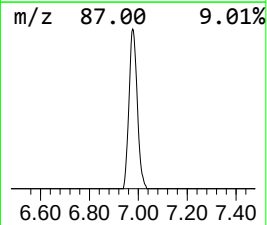
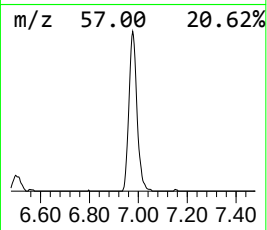
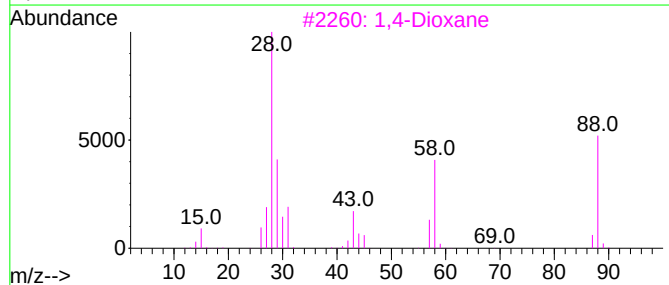
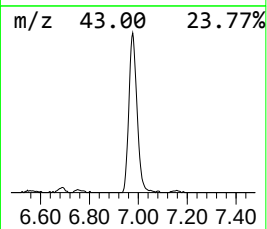
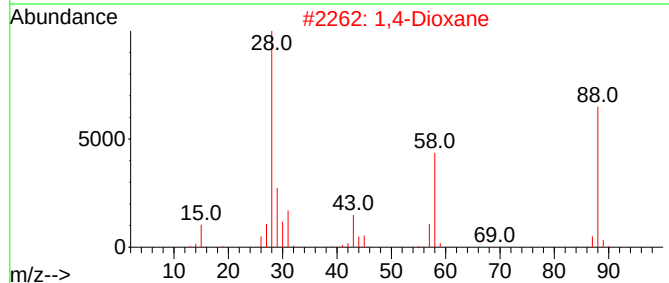
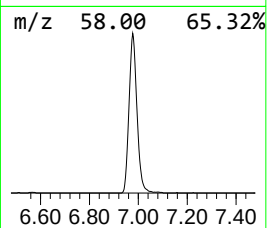
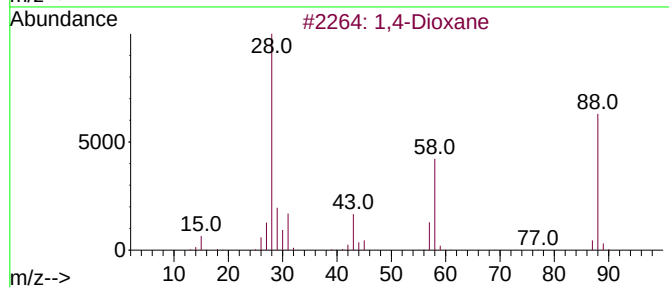
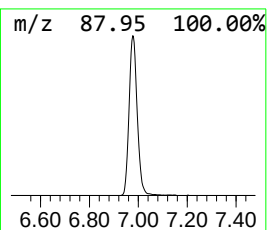
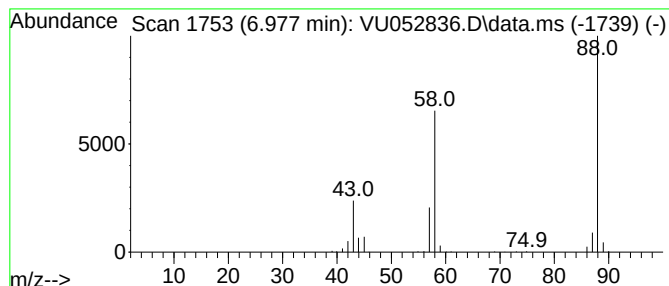
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Quant Title : VOC Analysis

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

Peak Number 5 1,4-Dioxane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.977	58.69 ug/L	459620	1,4-Difluorobenzene	6.244

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Dioxane	88	C4H8O2	000123-91-1	91
2			1,4-Dioxane	88	C4H8O2	000123-91-1	90
3			1,4-Dioxane	88	C4H8O2	000123-91-1	83
4			1,4-Dioxane	88	C4H8O2	000123-91-1	83
5			1,4-Dioxane	88	C4H8O2	000123-91-1	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012723\
Data File : VU052836.D
Acq On : 27 Jan 2023 11:07
Operator : JC/MD
Sample : 01316-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A44G8

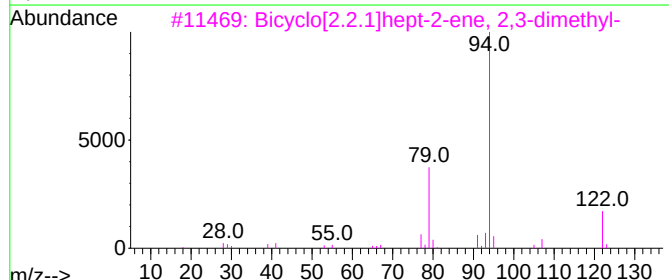
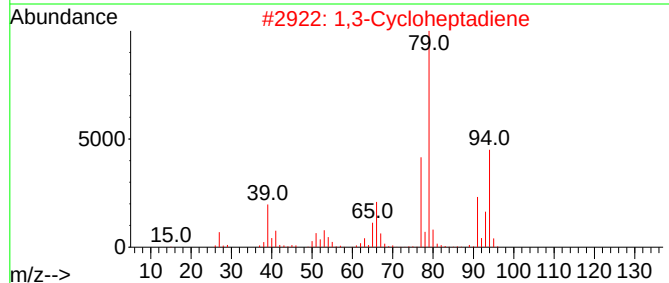
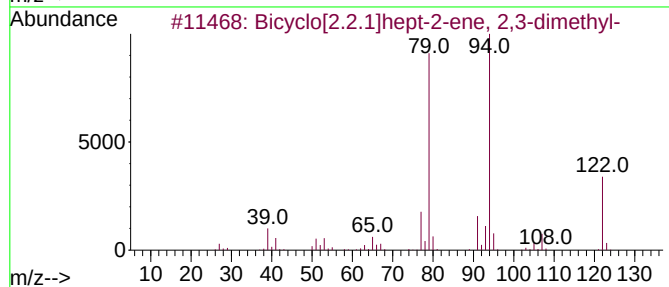
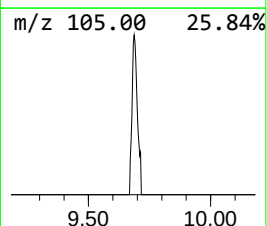
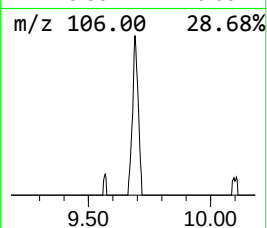
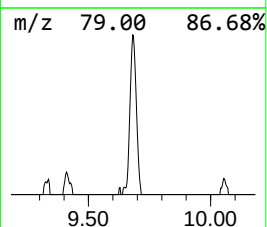
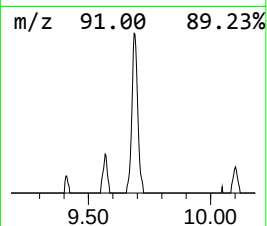
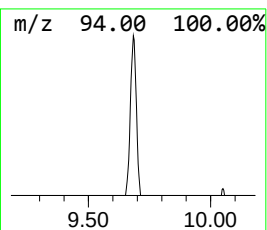
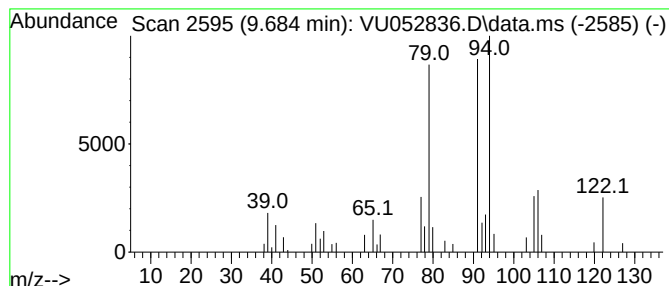
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Quant Title : VOC Analysis

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

Peak Number 7 Bicyclo[2.2.1]hept-2-ene, 2... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.684	2.81 ug/L	32255	Chlorobenzene-d5	9.414

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[2.2.1]hept-2-ene, 2,3-di...	122	C9H14	000529-16-8	58
2			1,3-Cycloheptadiene	94	C7H10	004054-38-0	58
3			Bicyclo[2.2.1]hept-2-ene, 2,3-di...	122	C9H14	000529-16-8	53
4			Cyclopentane, 1,3-bis(methylene)-	94	C7H10	059219-48-6	50
5			1,3,5-Heptatriene, (E,E)-	94	C7H10	017679-93-5	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012723\
Data File : VU052836.D
Acq On : 27 Jan 2023 11:07
Operator : JC/MD
Sample : 01316-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A44G8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM012623WMA.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
Ethyl ether	2.372	34.0	ug/L	266316	1	6.244	391540	50.0
1-Butanol, 3-me...	3.186	95.1	ug/L	744466	1	6.244	391540	50.0
Diisopropyl ether	3.990	4.7	ug/L	36415	1	6.244	391540	50.0
1,4-Dioxane	6.977	58.7	ug/L	459620	1	6.244	391540	50.0
Bicyclo[2.2.1]h...	9.684	2.8	ug/L	32255	2	9.414	572995	50.0