

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060623\
 Data File : VX036045.D
 Acq On : 06 Jun 2023 20:05
 Operator : JC/MD
 Sample : 02992-01 20X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 F6C08

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_X\Method\SFAMXML060623WMA.M

Title : VOC Analysis

Signal : TIC: VX036045.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	15	rVB	8907	9660	0.75%	0.068%
2	1.264	26	29	32	rBV	8899	8459	0.66%	0.059%
3	1.368	42	46	59	rVB	149729	184414	14.37%	1.297%
4	1.673	91	96	104	rBV	94016	140815	10.97%	0.990%
5	1.752	104	109	118	rVB	122854	171057	13.33%	1.203%
6	1.953	137	142	149	rVB	77723	104282	8.13%	0.733%
7	2.307	193	200	212	rBV	251984	420192	32.75%	2.955%
8	2.508	231	233	240	rVB2	700	973	0.08%	0.007%
9	2.569	240	243	244	rBV2	320	262	0.02%	0.002%
10	2.630	249	253	255	rBV3	480	795	0.06%	0.006%
11	2.776	271	277	281	rBV3	16306	36269	2.83%	0.255%
12	2.941	301	304	313	rVB3	4334	8393	0.65%	0.059%
13	3.099	322	330	344	rVB3	31647	72880	5.68%	0.512%
14	3.331	364	368	370	rBV2	282	428	0.03%	0.003%
15	3.447	379	387	396	rVV2	15998	36391	2.84%	0.256%
16	3.514	396	398	400	rVB2	331	270	0.02%	0.002%
17	3.556	400	405	408	rBV2	274	516	0.04%	0.004%
18	3.654	420	421	427	rVB2	268	281	0.02%	0.002%
19	3.953	467	470	471	rBV2	233	237	0.02%	0.002%
20	4.056	479	487	489	rBV5	1204	2602	0.20%	0.018%
21	4.197	505	510	511	rBV2	927	1194	0.09%	0.008%
22	4.300	517	527	540	rVB2	118688	341671	26.63%	2.402%
23	4.483	544	557	570	rBV2	221542	703822	54.85%	4.949%
24	5.056	639	651	671	rBV	155250	495397	38.61%	3.483%
25	5.379	702	704	705	rBV2	365	316	0.02%	0.002%
26	5.471	707	719	734	rVV	232242	721362	56.22%	5.072%
27	5.843	769	780	789	rBV7	7600	25815	2.01%	0.182%
28	5.971	789	801	807	rBV2	426784	1283151	100.00%	9.023%
29	6.263	841	849	855	rBV3	6752	18106	1.41%	0.127%
30	6.355	857	864	873	rVB4	11263	31371	2.44%	0.221%
31	6.611	901	906	915	rBV5	1907	4750	0.37%	0.033%
32	6.757	921	930	948	rBV	315692	758833	59.14%	5.336%
33	7.123	980	990	1008	rVV	387831	844534	65.82%	5.938%
34	7.306	1011	1020	1026	rVV	264826	575119	44.82%	4.044%
35	7.379	1027	1032	1043	rVB	160565	350975	27.35%	2.468%
36	7.611	1068	1070	1071	rVB2	392	240	0.02%	0.002%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML060623WMA.M
 Title : VOC Analysis

37	7.659	1071	1078	1085	rBV3	4972	9392	0.73%	0.066%
38	7.769	1090	1096	1104	rVB6	1163	2007	0.16%	0.014%
39	7.921	1119	1121	1122	rBV	346	237	0.02%	0.002%
40	8.104	1147	1151	1152	rBV3	476	513	0.04%	0.004%
41	8.232	1170	1172	1177	rBV2	236	268	0.02%	0.002%
42	8.324	1178	1187	1200	rVV	160115	260543	20.30%	1.832%
43	8.434	1204	1205	1209	rVB4	893	795	0.06%	0.006%
44	8.592	1225	1231	1234	rBV5	5487	10811	0.84%	0.076%
45	8.647	1234	1240	1248	rVV	653231	1012969	78.94%	7.123%
46	8.720	1249	1252	1256	rVV2	8594	12954	1.01%	0.091%
47	8.769	1258	1260	1268	rVB2	3783	5326	0.42%	0.037%
48	8.952	1284	1290	1308	rVB	109586	176351	13.74%	1.240%
49	9.098	1310	1314	1319	rBV3	3211	5138	0.40%	0.036%
50	9.275	1336	1343	1349	rBV	131414	195924	15.27%	1.378%
51	9.385	1355	1361	1372	rBV	410802	587437	45.78%	4.131%
52	9.561	1385	1390	1396	rVB	5359	7926	0.62%	0.056%
53	9.610	1396	1398	1402	rVB3	612	657	0.05%	0.005%
54	9.830	1431	1434	1435	rBV	251	256	0.02%	0.002%
55	9.945	1451	1453	1456	rBV	377	276	0.02%	0.002%
56	10.055	1465	1471	1480	rBV	647496	896492	69.87%	6.304%
57	10.195	1488	1494	1500	rBV	148151	195331	15.22%	1.373%
58	10.299	1504	1511	1523	rVB	437596	589880	45.97%	4.148%
59	10.586	1555	1558	1559	rBV2	398	441	0.03%	0.003%
60	10.640	1562	1567	1575	rVB	76037	97771	7.62%	0.687%
61	10.781	1587	1590	1595	rBV2	583	623	0.05%	0.004%
62	10.848	1597	1601	1603	rBV	492	699	0.05%	0.005%
63	10.964	1615	1620	1627	rVB	25054	31481	2.45%	0.221%
64	11.086	1637	1640	1644	rBV2	607	821	0.06%	0.006%
65	11.189	1649	1657	1670	rBV	434493	579612	45.17%	4.076%
66	11.305	1672	1676	1682	rVB	17312	21322	1.66%	0.150%
67	11.378	1683	1688	1696	rBV	59848	98679	7.69%	0.694%
68	11.451	1696	1700	1704	rVB	45290	53633	4.18%	0.377%
69	11.610	1721	1726	1733	rBV	22647	29347	2.29%	0.206%
70	11.707	1740	1742	1744	rBV2	874	1005	0.08%	0.007%
71	11.750	1744	1749	1756	rVB	105315	126829	9.88%	0.892%
72	11.866	1765	1768	1769	rBV3	1297	1328	0.10%	0.009%
73	11.939	1778	1780	1781	rBV	428	357	0.03%	0.003%
74	11.970	1781	1785	1788	rVV2	4768	5575	0.43%	0.039%
75	12.018	1788	1793	1800	rVV	682827	864377	67.36%	6.078%
76	12.085	1800	1804	1813	rVV	62106	77156	6.01%	0.543%

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Integration Parameters: LSCINT.P

Integrator: RTE

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 Title : VOC Analysis

77	12.177	1816	1819	1823	rVB3	1148	1296	0.10%	0.009%
78	12.244	1823	1830	1833	rBV	8342	11384	0.89%	0.080%
79	12.317	1837	1842	1853	rVB	645148	843977	65.77%	5.934%
80	12.463	1863	1866	1872	rVB3	2181	2512	0.20%	0.018%
81	12.530	1872	1877	1879	rBV2	2958	3485	0.27%	0.025%
82	12.610	1887	1890	1895	rBV2	2393	3130	0.24%	0.022%
83	12.707	1902	1906	1910	rBV5	2595	4029	0.31%	0.028%
84	12.847	1925	1929	1932	rBV3	1882	2323	0.18%	0.016%
85	12.921	1939	1941	1944	rBV2	846	1012	0.08%	0.007%
86	12.963	1945	1948	1953	rVB2	1952	2214	0.17%	0.016%
87	13.116	1969	1973	1974	rBV2	347	460	0.04%	0.003%
88	13.286	1996	2001	2006	rBV3	2065	2817	0.22%	0.020%
89	13.420	2021	2023	2025	rVB2	868	703	0.05%	0.005%
90	13.585	2048	2050	2054	rVB2	508	587	0.05%	0.004%
91	13.774	2077	2081	2087	rVV	13172	17758	1.38%	0.125%
92	14.292	2164	2166	2170	rBV3	326	391	0.03%	0.003%
93	14.426	2183	2188	2189	rBV2	293	467	0.04%	0.003%
94	14.634	2218	2222	2227	rBV4	1379	2038	0.16%	0.014%
95	14.780	2244	2246	2249	rBV3	656	658	0.05%	0.005%
96	14.829	2252	2254	2256	rVV	450	251	0.02%	0.002%
97	15.432	2351	2353	2354	rBV2	472	276	0.02%	0.002%
98	15.524	2366	2368	2369	rBV2	508	359	0.03%	0.003%
99	15.646	2386	2388	2390	rVB2	845	485	0.04%	0.003%
100	16.475	2523	2524	2527	rVB2	863	642	0.05%	0.005%

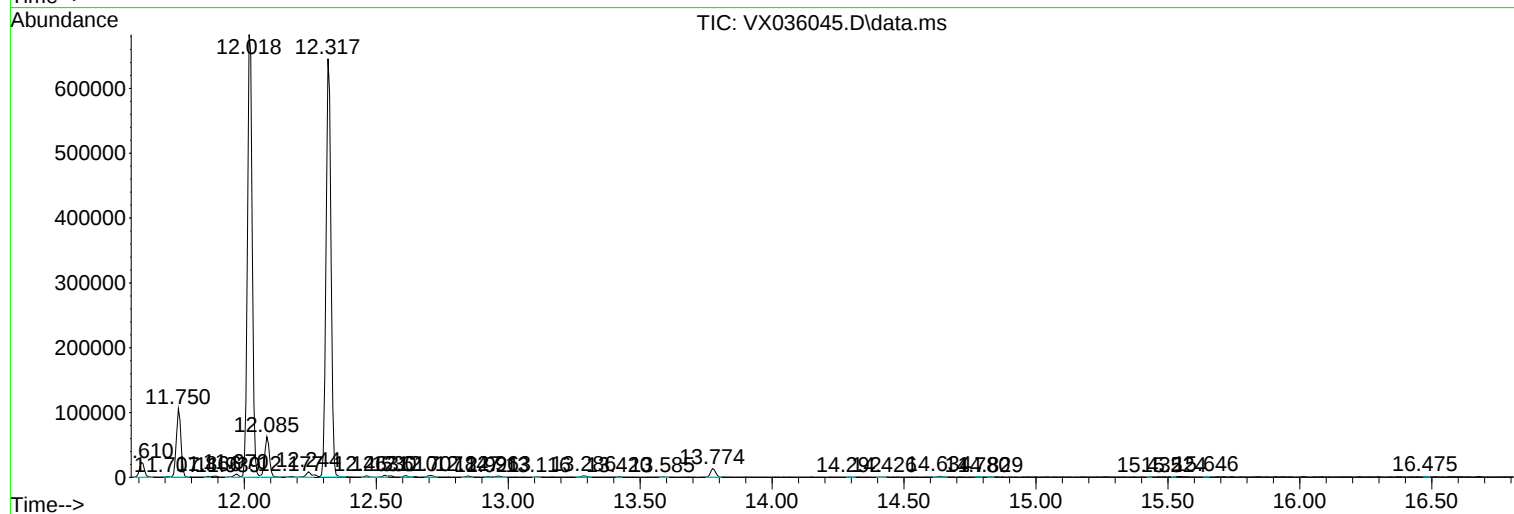
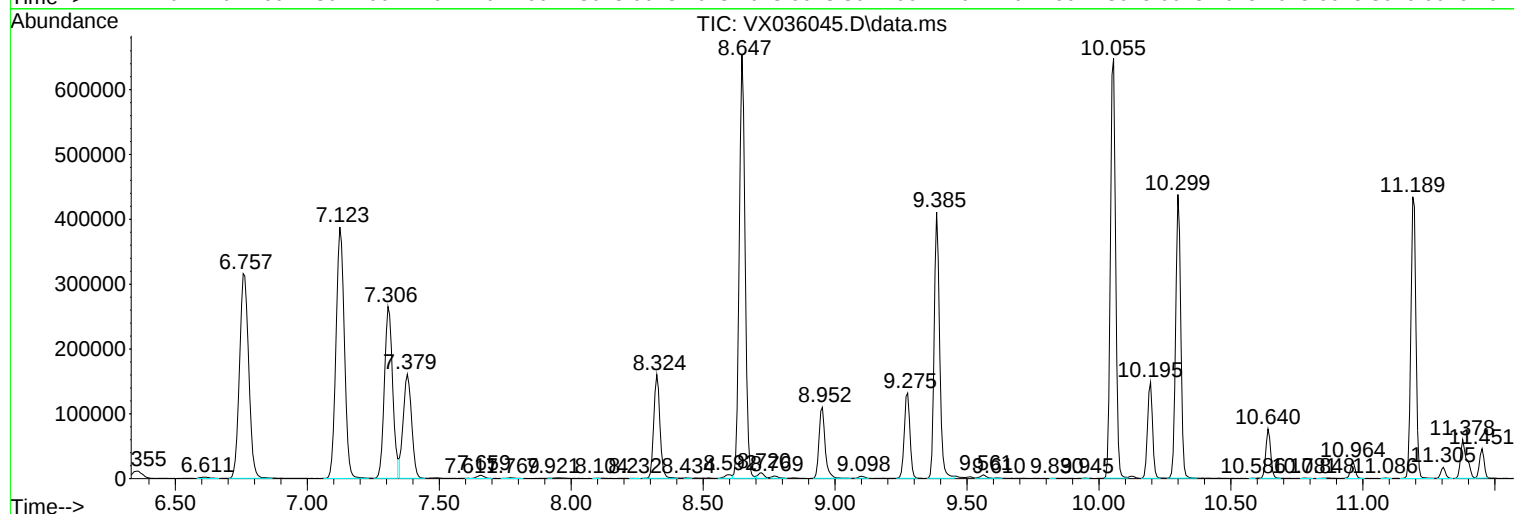
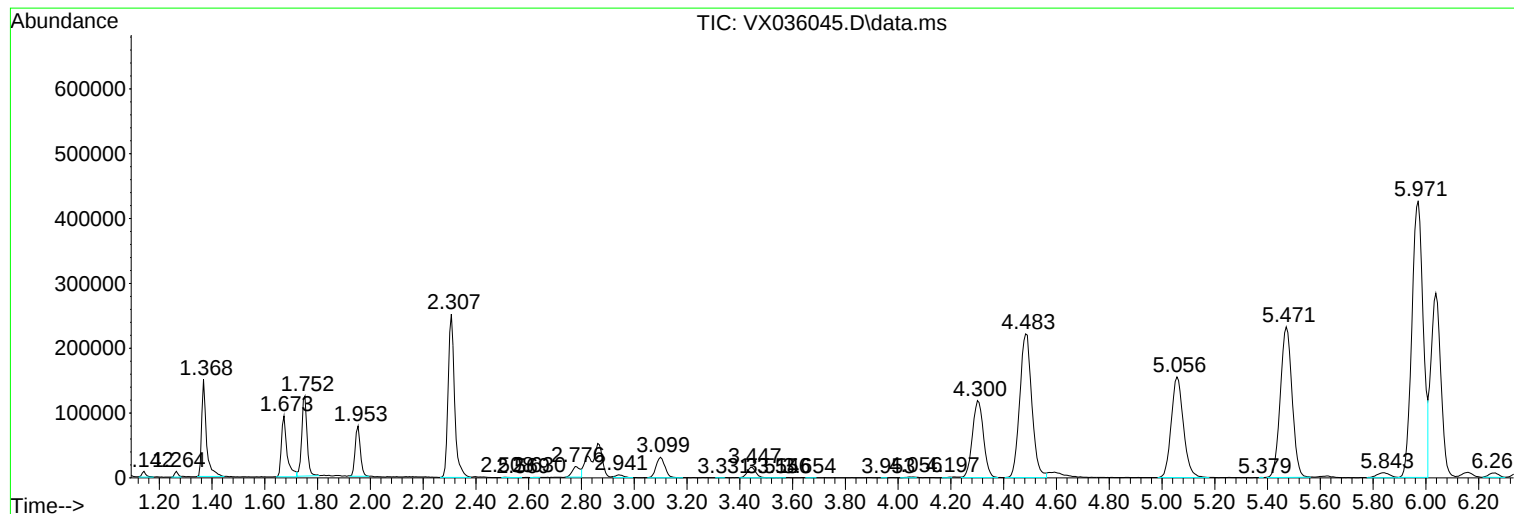
Sum of corrected areas: 14221625

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ALS Vial : 29 Sample Multiplier: 1

Instrument :
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ClientSampleId :
F6C08

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML060623WMA.M
Quant Title : VOC Analysis

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



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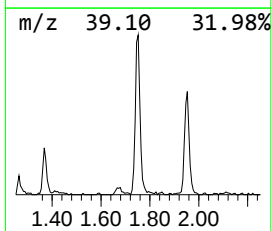
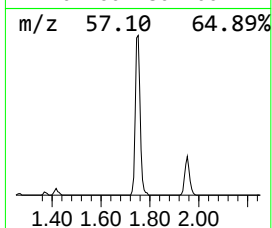
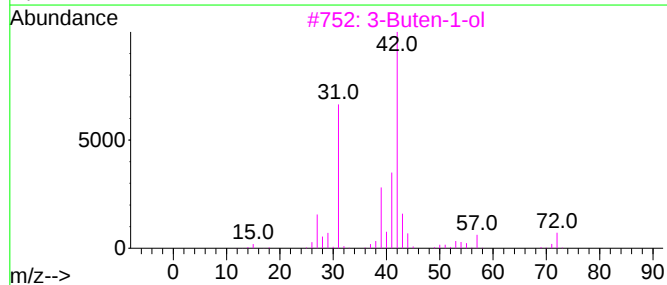
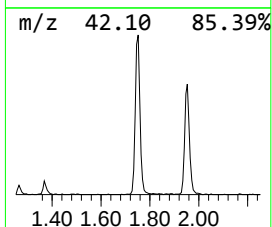
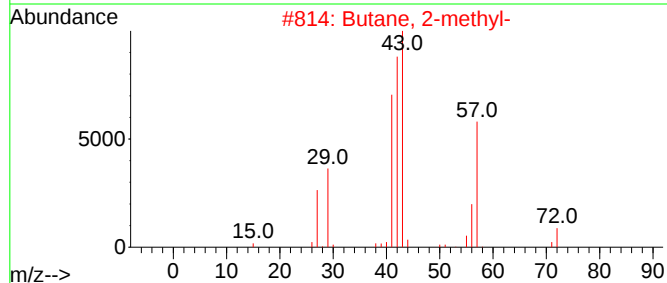
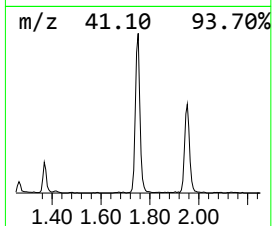
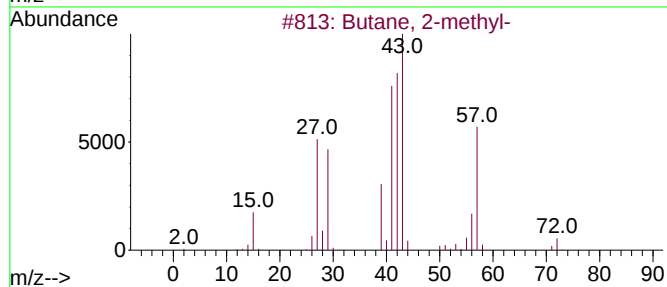
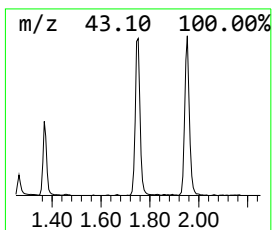
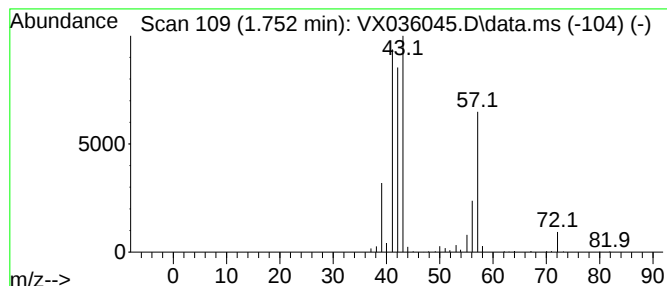
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML060623WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	11.27 ug/L	171057	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-			72	C5H12	000078-78-4	90
2	Butane, 2-methyl-			72	C5H12	000078-78-4	90
3	3-Buten-1-ol			72	C4H8O	000627-27-0	47
4	Pentane			72	C5H12	000109-66-0	33
5	1-Butene			56	C4H8	000106-98-9	9



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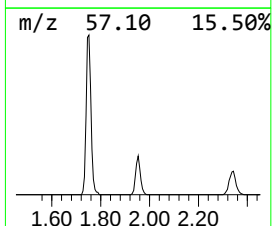
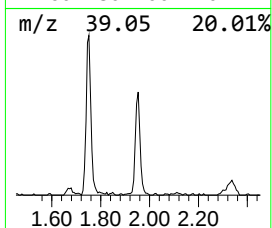
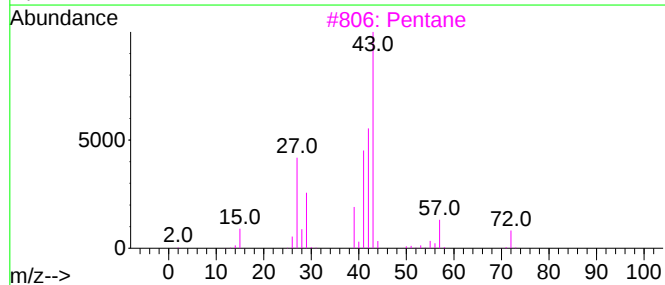
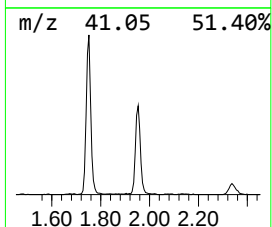
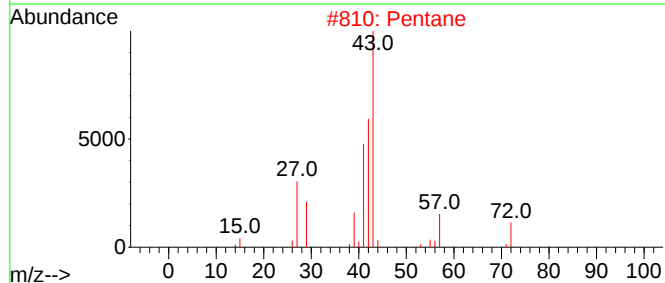
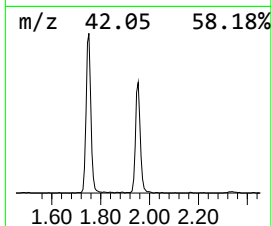
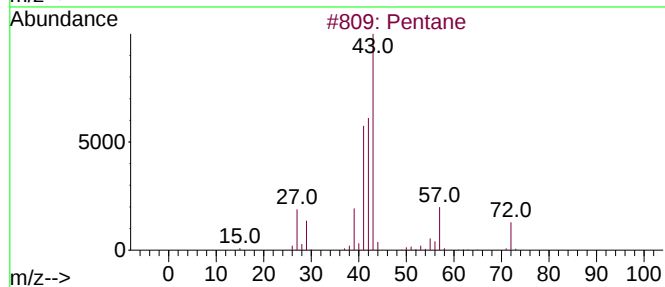
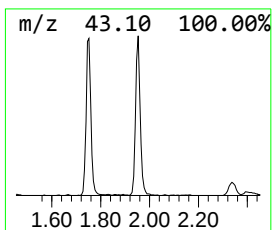
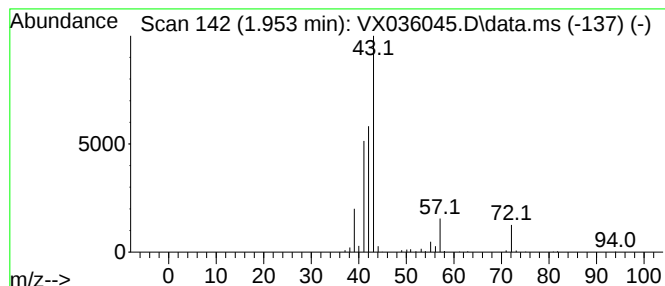
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML060623WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.953	6.87 ug/L	104282	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane			72	C5H12	000109-66-0	91
2	Pentane			72	C5H12	000109-66-0	90
3	Pentane			72	C5H12	000109-66-0	90
4	Pentane			72	C5H12	000109-66-0	86
5	Pentane			72	C5H12	000109-66-0	64



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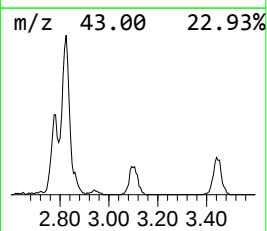
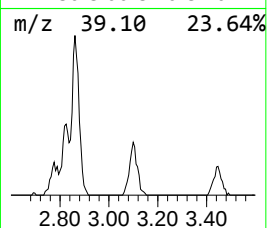
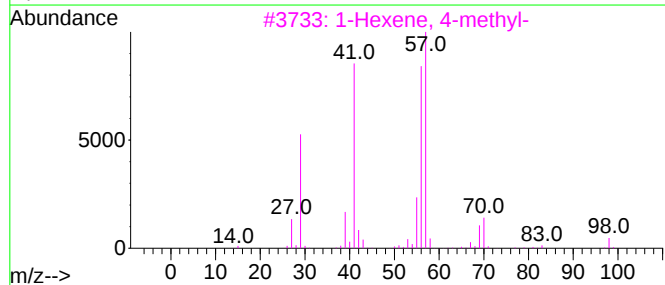
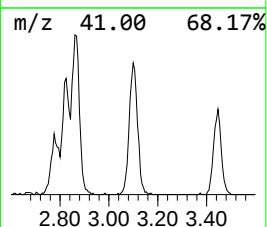
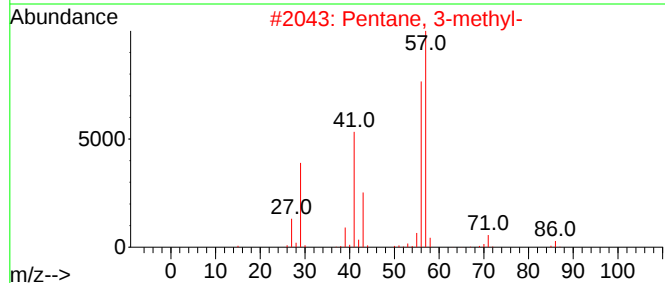
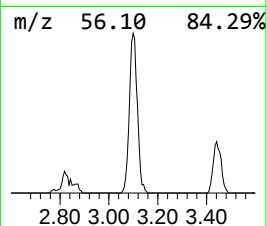
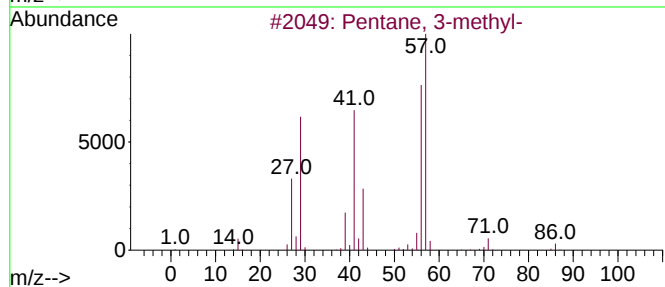
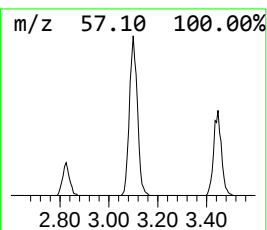
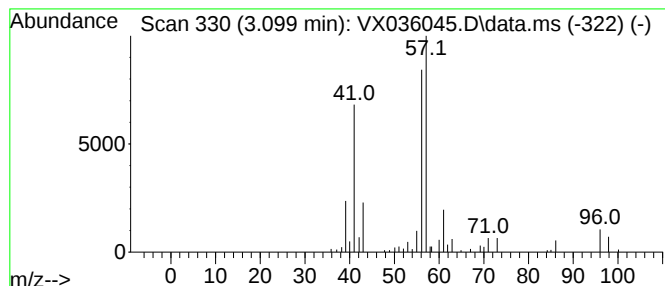
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML060623WMA.M
Quant Title : VOC Analysis

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.
3.099	4.80 ug/L	72880	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	58
2			Pentane, 3-methyl-	86	C6H14	000096-14-0	58
3			1-Hexene, 4-methyl-	98	C7H14	003769-23-1	52
4			Pentane, 3-methyl-	86	C6H14	000096-14-0	52
5			Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060623\
Data File : VX036045.D
Acq On : 06 Jun 2023 20:05
Operator : JC/MD
Sample : 02992-01 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
F6C08

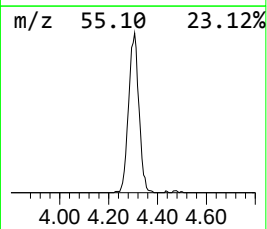
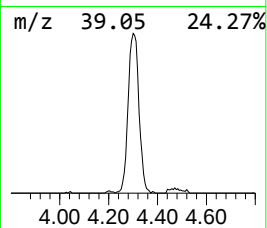
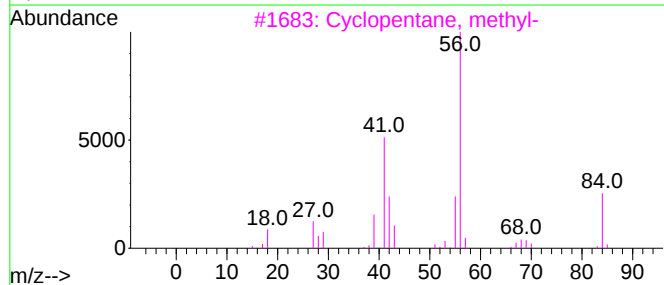
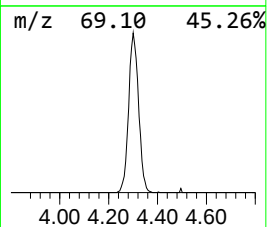
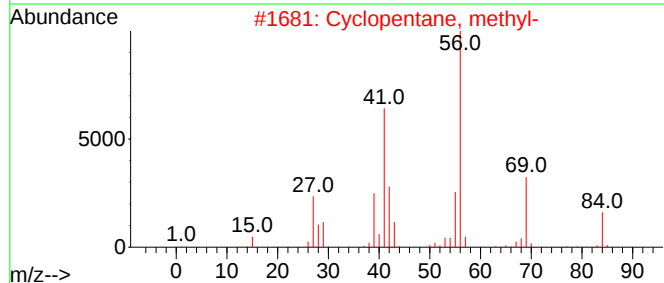
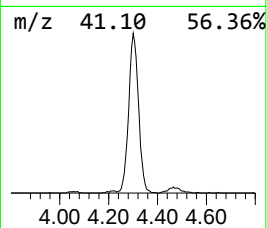
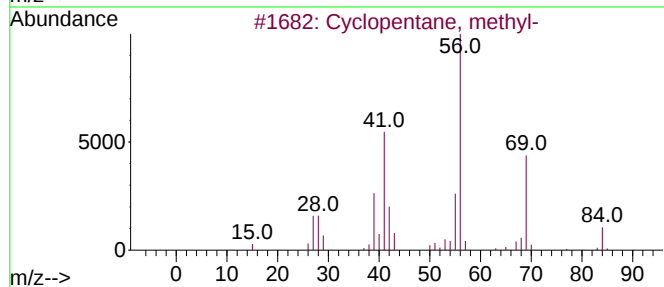
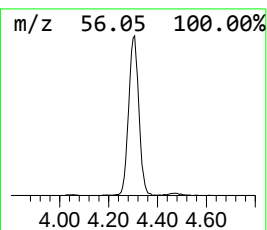
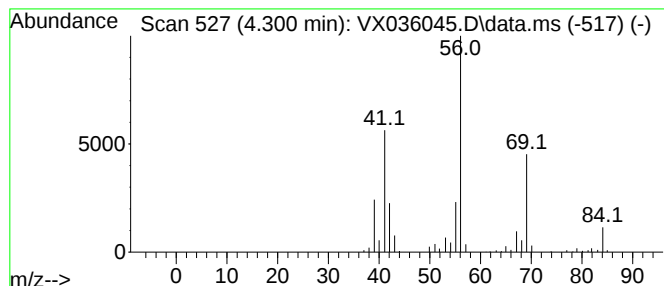
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Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Cyclic4.300 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.300	22.51 ug/L	341671	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2			Cyclopentane, methyl-	84	C6H12	000096-37-7	86
3			Cyclopentane, methyl-	84	C6H12	000096-37-7	72
4			Cyclohexane	84	C6H12	000110-82-7	72
5			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060623\
Data File : VX036045.D
Acq On : 06 Jun 2023 20:05
Operator : JC/MD
Sample : 02992-01 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
F6C08

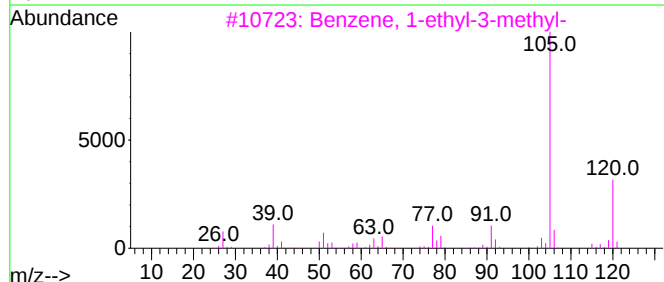
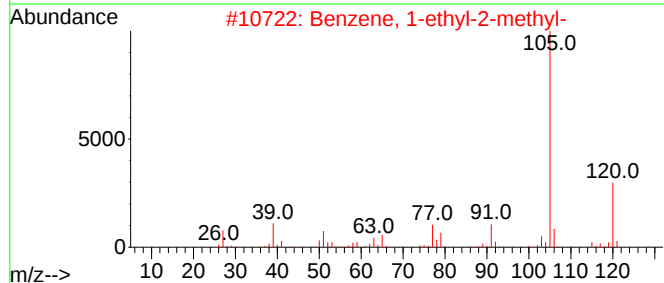
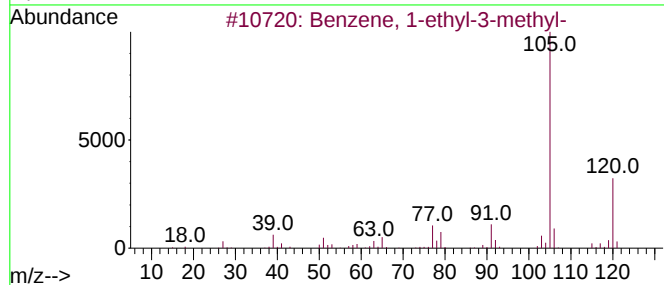
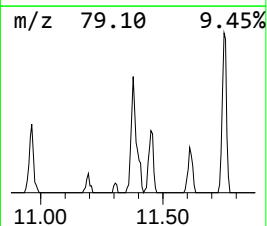
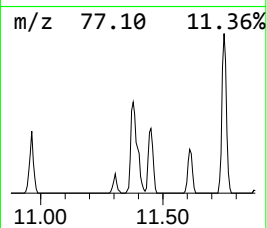
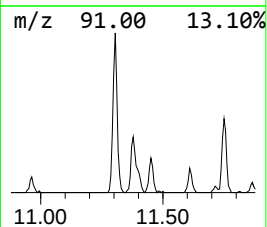
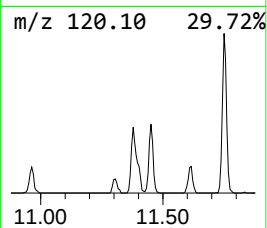
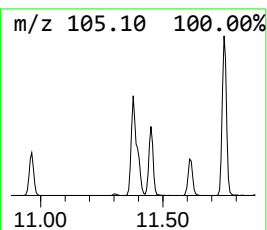
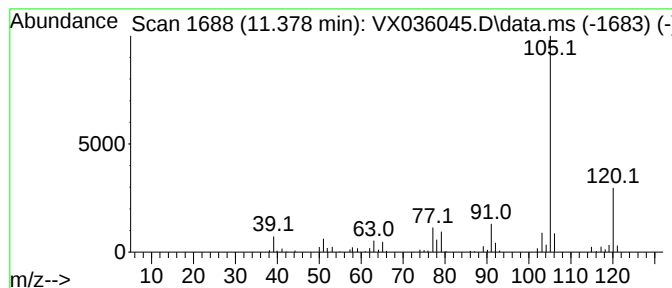
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Quant Title : VOC Analysis

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

Peak Number 6 Benzene, 1-ethyl-3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	5.71 ug/L	98679	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	97
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
4			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060623\
Data File : VX036045.D
Acq On : 06 Jun 2023 20:05
Operator : JC/MD
Sample : 02992-01 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
F6C08

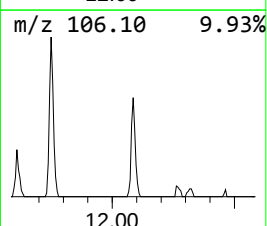
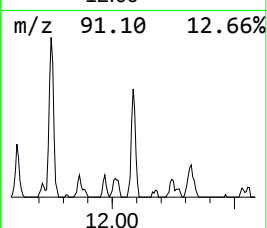
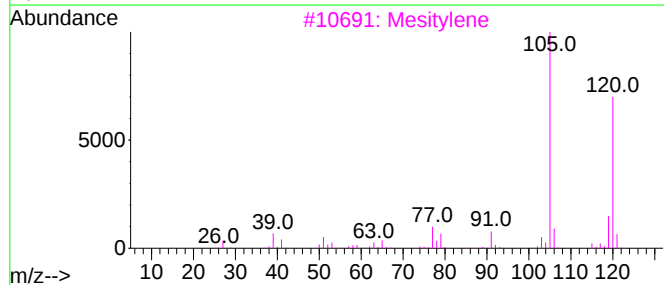
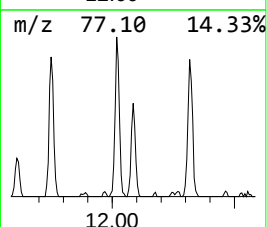
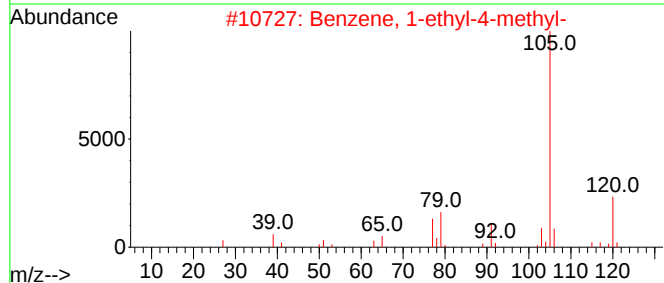
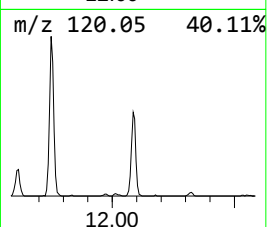
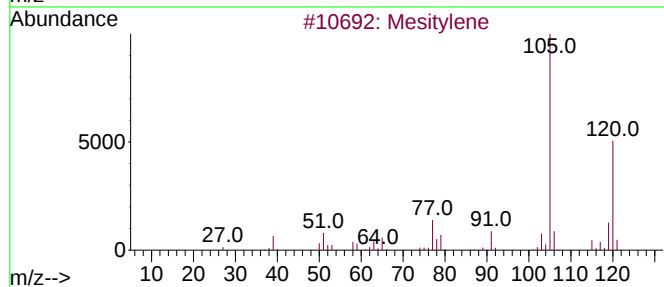
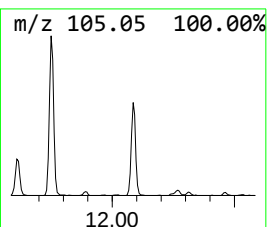
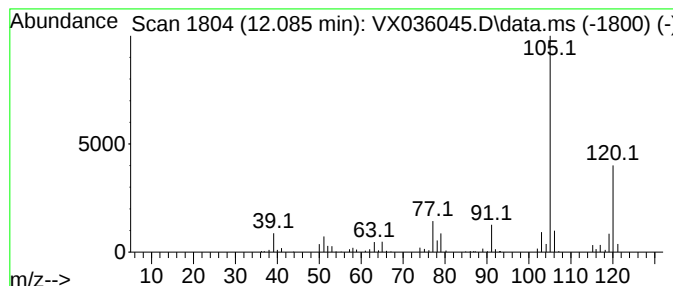
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML060623WMA.M
Quant Title : VOC Analysis

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

Peak Number 7 Benzene, 1-ethyl-4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	4.46 ug/L	77156	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	94
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060623\
Data File : VX036045.D
Acq On : 06 Jun 2023 20:05
Operator : JC/MD
Sample : 02992-01 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
F6C08

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML060623WMA.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
(DEL) Alkane: S...	1.752	11.3	ug/L	171057	1	6.757	758833	50.0
(DEL) Alkane: S...	1.953	6.9	ug/L	104282	1	6.757	758833	50.0
(DEL) Alkane: S...	3.099	4.8	ug/L	72880	1	6.757	758833	50.0
(DEL) Alkane: C...	4.300	22.5	ug/L	341671	1	6.757	758833	50.0
Benzene, 1-ethy...	11.378	5.7	ug/L	98679	3	12.024	864377	50.0
Benzene, 1-ethy...	12.085	4.5	ug/L	77156	3	12.024	864377	50.0