

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080622\
 Data File : VX030493.D
 Acq On : 07 Aug 2022 03:16
 Operator : JC/MD
 Sample : N4021-11
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 F5D67

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\SFAMXML080422WMA.M
 Title : VOC Analysis

Signal : TIC: VX030493.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	43	47	58	rVB	2277001	2443476	86.00%	17.559%
2	1.666	91	95	103	rVB	93639	114583	4.03%	0.823%
3	1.953	139	142	149	rVB	8908	12295	0.43%	0.088%
4	2.306	194	200	211	rVB	216239	347493	12.23%	2.497%
5	2.392	211	214	216	rBV3	930	1039	0.04%	0.007%
6	2.654	253	257	260	rVB3	475	797	0.03%	0.006%
7	2.678	260	261	263	rBV2	712	572	0.02%	0.004%
8	2.782	271	278	281	rBV2	12153	26040	0.92%	0.187%
9	2.825	281	285	290	rVV2	22685	44744	1.57%	0.322%
10	2.977	309	310	313	rBV3	775	1003	0.04%	0.007%
11	3.099	322	330	341	rBV2	122295	256286	9.02%	1.842%
12	3.331	359	368	372	rBV5	2077	4683	0.16%	0.034%
13	3.446	379	387	394	rBV3	5600	12336	0.43%	0.089%
14	3.568	402	407	408	rBV4	1057	1377	0.05%	0.010%
15	3.727	428	433	439	rBV4	2381	5175	0.18%	0.037%
16	3.776	439	441	442	rVB2	651	405	0.01%	0.003%
17	3.794	442	444	446	rBV2	452	548	0.02%	0.004%
18	3.837	448	451	456	rVV3	819	1559	0.05%	0.011%
19	3.898	459	461	463	rVV3	574	520	0.02%	0.004%
20	3.940	466	468	471	rBV2	437	462	0.02%	0.003%
21	4.038	481	484	485	rBV3	997	1192	0.04%	0.009%
22	4.099	492	494	497	rVB3	1028	895	0.03%	0.006%
23	4.215	504	513	520	rBV6	7422	23107	0.81%	0.166%
24	4.306	520	528	541	rVB2	64849	188289	6.63%	1.353%
25	4.397	541	543	545	rBV	763	768	0.03%	0.006%
26	4.495	546	559	578	rBV2	1008690	2841199	100.00%	20.417%
27	5.068	640	653	671	rBV	135963	420615	14.80%	3.023%
28	5.348	694	699	700	rBV4	451	742	0.03%	0.005%
29	5.391	703	706	708	rBV4	1369	1608	0.06%	0.012%
30	5.477	711	720	733	rVB2	57165	178880	6.30%	1.285%
31	5.623	736	744	757	rVB3	33855	110519	3.89%	0.794%
32	5.714	757	759	763	rVB3	544	680	0.02%	0.005%
33	5.836	767	779	789	rBV7	13457	46001	1.62%	0.331%
34	5.976	789	802	811	rBV2	341781	1018111	35.83%	7.316%
35	6.165	827	833	840	rBV7	10222	31424	1.11%	0.226%
36	6.367	858	866	876	rVB5	13412	38261	1.35%	0.275%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
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37	6.476	881	884	888	rBV3	690	1154	0.04%	0.008%
38	6.556	895	897	898	rBV	613	470	0.02%	0.003%
39	6.769	922	932	944	rBV	294627	716311	25.21%	5.147%
40	6.982	963	967	968	rBV3	1150	1512	0.05%	0.011%
41	7.037	975	976	978	rBV	550	407	0.01%	0.003%
42	7.055	978	979	981	rBV2	492	492	0.02%	0.004%
43	7.129	982	991	998	rBV6	13481	40041	1.41%	0.288%
44	7.312	1012	1021	1028	rBV	212531	473567	16.67%	3.403%
45	7.507	1047	1053	1057	rVB7	1431	3216	0.11%	0.023%
46	7.659	1072	1078	1084	rBV4	7462	15312	0.54%	0.110%
47	7.775	1088	1097	1104	rBV5	2056	5333	0.19%	0.038%
48	7.866	1104	1112	1113	rBV4	4113	8347	0.29%	0.060%
49	7.964	1123	1128	1130	rBV5	2397	4235	0.15%	0.030%
50	8.110	1145	1152	1158	rBV3	4831	10124	0.36%	0.073%
51	8.250	1173	1175	1180	rVB2	377	474	0.02%	0.003%
52	8.330	1180	1188	1200	rBV	124267	210718	7.42%	1.514%
53	8.519	1213	1219	1224	rBV5	3025	6485	0.23%	0.047%
54	8.604	1227	1233	1235	rBV4	5064	8322	0.29%	0.060%
55	8.653	1235	1241	1249	rVB	511169	782115	27.53%	5.620%
56	8.823	1267	1269	1271	rBV2	942	573	0.02%	0.004%
57	8.854	1271	1274	1276	rVV2	799	782	0.03%	0.006%
58	8.958	1285	1291	1301	rBV	87834	137790	4.85%	0.990%
59	9.067	1307	1309	1311	rBV	1197	1137	0.04%	0.008%
60	9.104	1311	1315	1321	rVB6	4234	6857	0.24%	0.049%
61	9.275	1341	1343	1348	rVV3	923	1305	0.05%	0.009%
62	9.390	1356	1362	1372	rBV	410555	576539	20.29%	4.143%
63	9.506	1378	1381	1382	rBV3	1201	1372	0.05%	0.010%
64	9.970	1455	1457	1461	rBV3	592	571	0.02%	0.004%
65	10.055	1465	1471	1481	rBV	600021	825528	29.06%	5.932%
66	10.201	1489	1495	1499	rVB3	2197	3675	0.13%	0.026%
67	10.250	1501	1503	1504	rVV2	857	466	0.02%	0.003%
68	10.311	1509	1513	1519	rVB2	5182	7989	0.28%	0.057%
69	10.445	1533	1535	1537	rVB2	758	529	0.02%	0.004%
70	10.543	1548	1551	1555	rBV	541	893	0.03%	0.006%
71	10.591	1557	1559	1562	rVV2	495	559	0.02%	0.004%
72	10.646	1565	1568	1572	rVV3	1954	2275	0.08%	0.016%
73	10.750	1582	1585	1589	rVB3	413	556	0.02%	0.004%
74	10.793	1589	1592	1593	rBV2	648	569	0.02%	0.004%
75	10.969	1616	1621	1624	rBV3	2392	2704	0.10%	0.019%
76	11.000	1624	1626	1631	rVB2	489	432	0.02%	0.003%

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77	11.152	1649	1651	1652	rBV2	454	397	0.01%	0.003%
78	11.195	1652	1658	1665	rBV	372351	462253	16.27%	3.322%
79	11.323	1675	1679	1680	rBV2	535	561	0.02%	0.004%
80	11.396	1687	1691	1692	rBV	533	578	0.02%	0.004%
81	11.475	1702	1704	1705	rVV2	617	442	0.02%	0.003%
82	11.494	1705	1707	1709	rVV	679	662	0.02%	0.005%
83	11.835	1760	1763	1766	rBV	506	653	0.02%	0.005%
84	11.896	1769	1773	1779	rVV4	2160	3501	0.12%	0.025%
85	12.024	1788	1794	1803	rBV	630205	746689	26.28%	5.366%
86	12.177	1817	1819	1822	rBV3	682	677	0.02%	0.005%
87	12.225	1824	1827	1830	rBV3	723	1157	0.04%	0.008%
88	12.323	1837	1843	1850	rBV	514244	651532	22.93%	4.682%
89	12.585	1884	1886	1891	rVB2	502	706	0.02%	0.005%
90	12.640	1891	1895	1900	rBV2	632	1040	0.04%	0.007%
91	12.774	1913	1917	1919	rBV2	503	547	0.02%	0.004%
92	13.054	1960	1963	1965	rBV2	448	420	0.01%	0.003%
93	13.121	1970	1974	1975	rBV2	363	567	0.02%	0.004%
94	13.396	2017	2019	2023	rVB	602	659	0.02%	0.005%
95	13.481	2029	2033	2036	rBV2	477	550	0.02%	0.004%
96	14.408	2182	2185	2187	rBV	638	574	0.02%	0.004%
97	14.835	2251	2255	2256	rBV3	611	737	0.03%	0.005%
98	15.054	2288	2291	2293	rBV2	557	560	0.02%	0.004%
99	16.200	2477	2479	2480	rBV	675	422	0.01%	0.003%
100	16.377	2506	2508	2510	rBV3	603	450	0.02%	0.003%

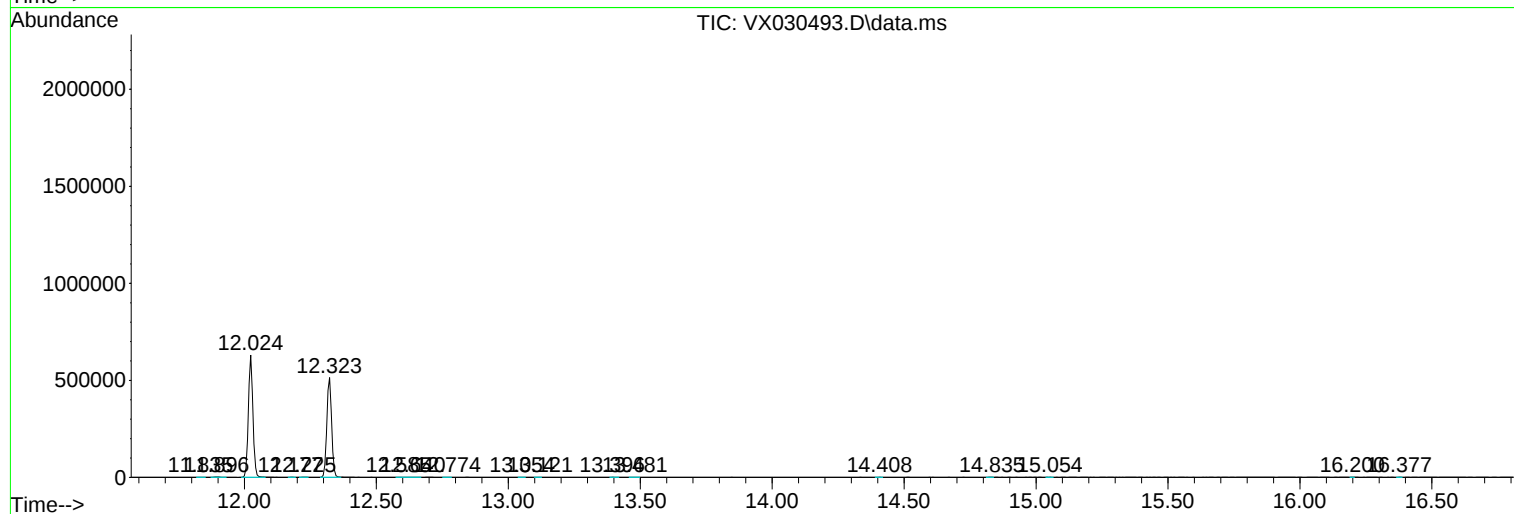
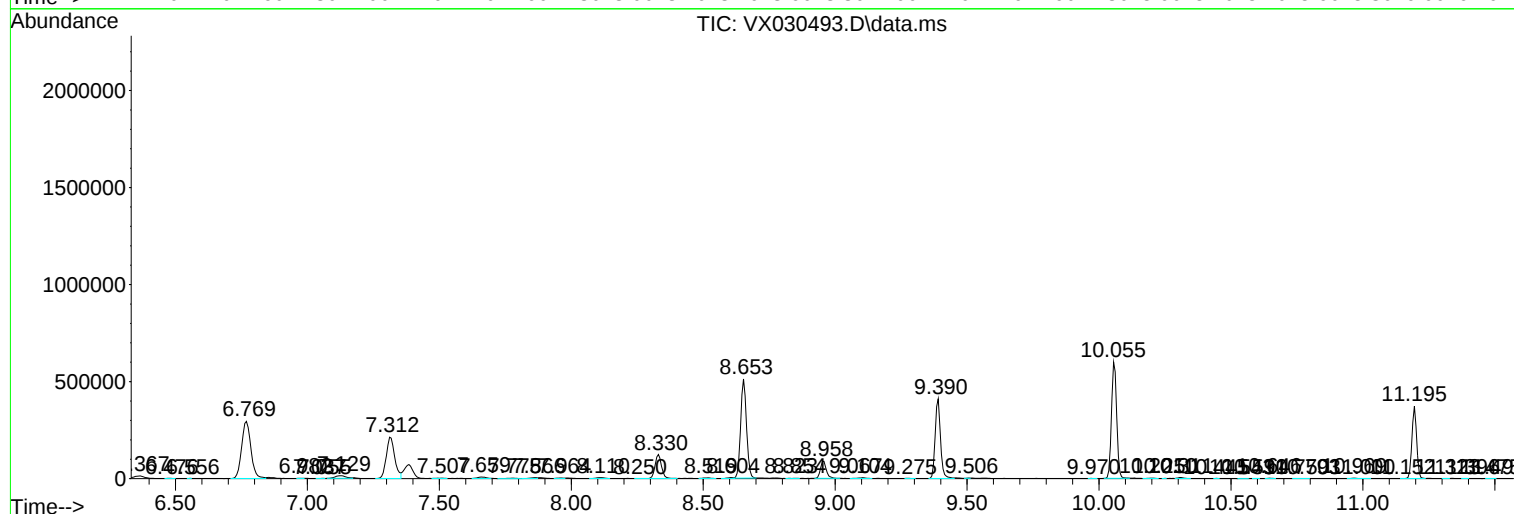
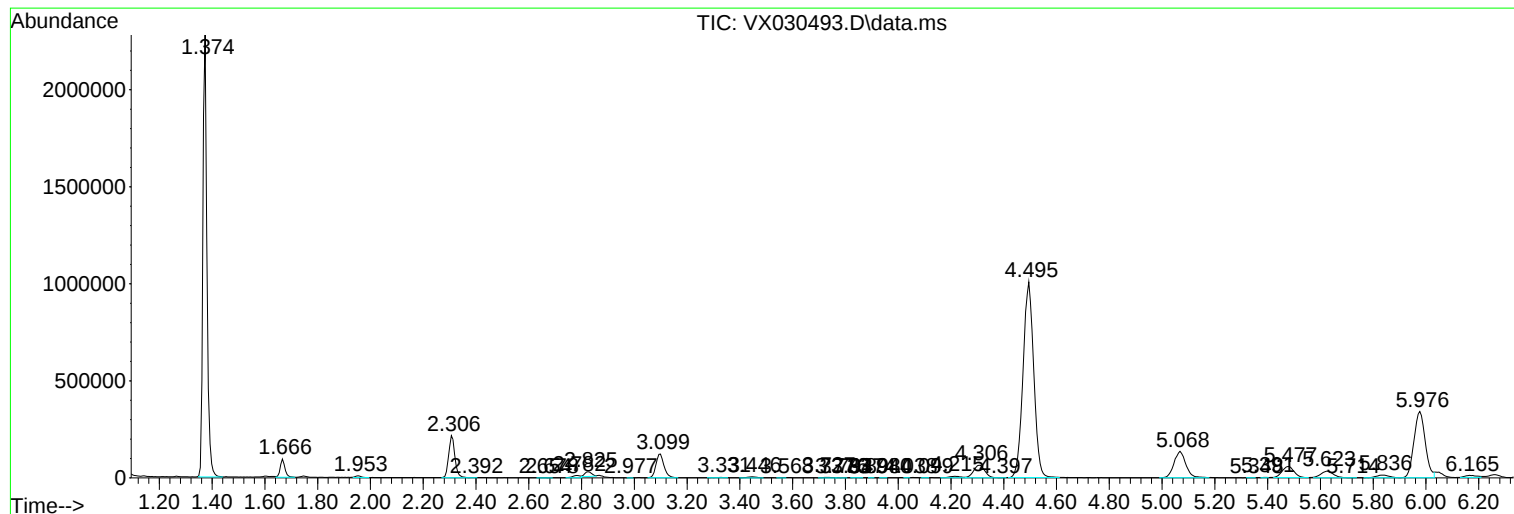
Sum of corrected areas: 13915754

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Instrument :
MSVOA_X
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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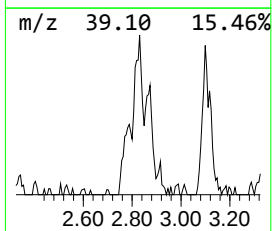
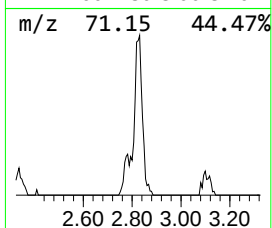
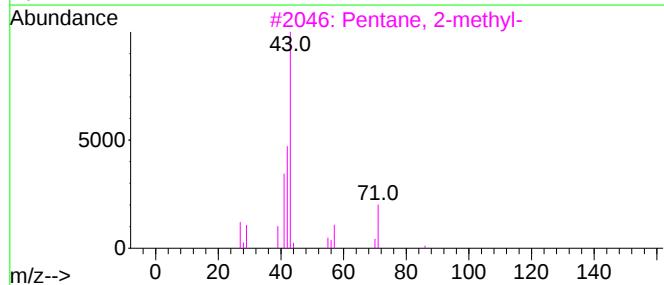
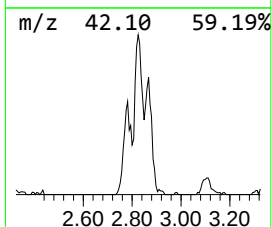
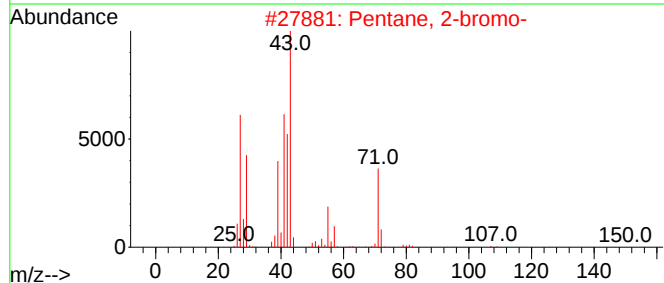
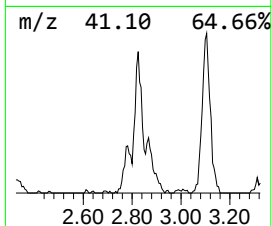
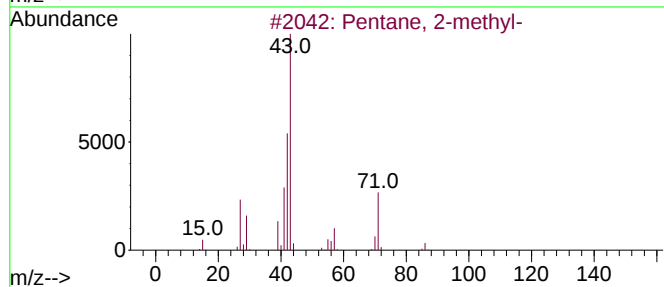
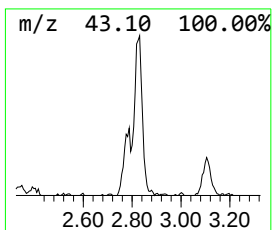
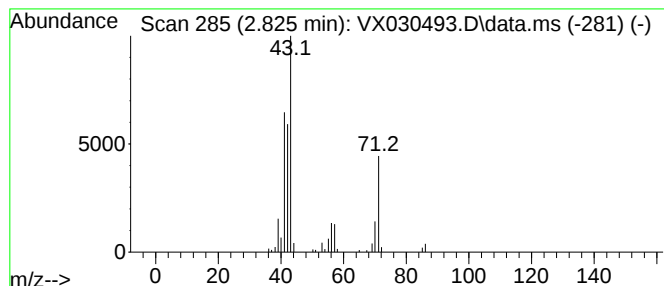
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.825	3.12 ug/L	44744	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	86
2			Pentane, 2-bromo-	150	C5H11Br	000107-81-3	59
3			Pentane, 2-methyl-	86	C6H14	000107-83-5	59
4			Pentane, 2-methyl-	86	C6H14	000107-83-5	56
5			Pentane, 2-methyl-	86	C6H14	000107-83-5	50



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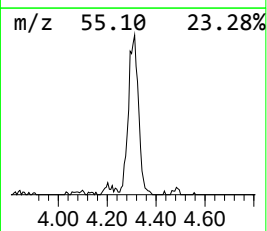
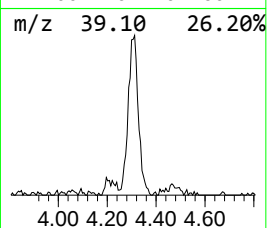
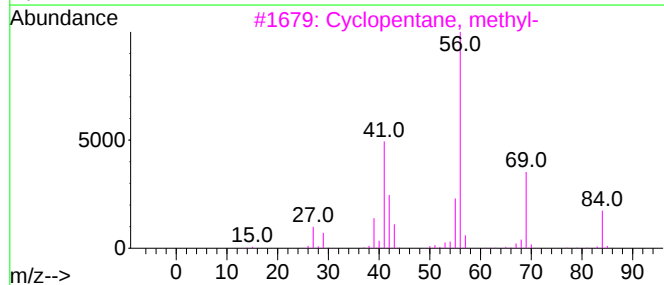
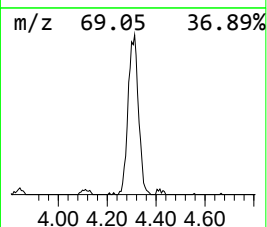
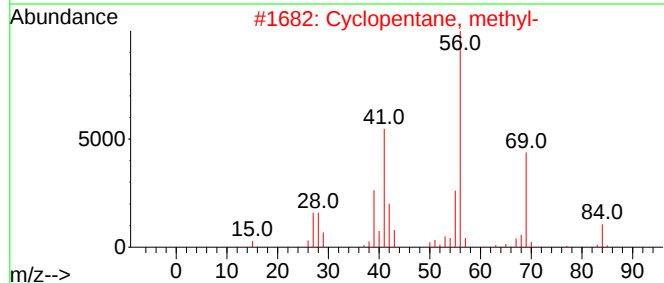
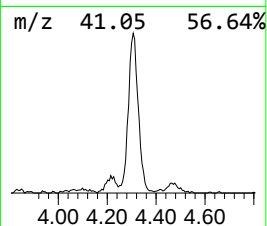
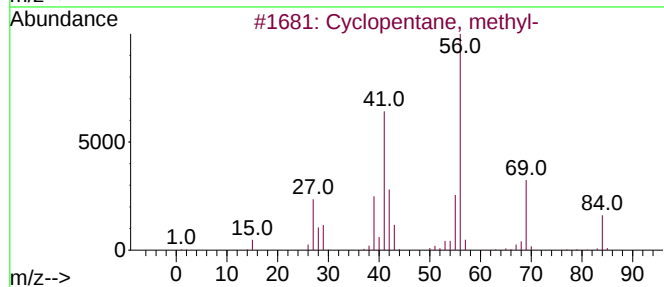
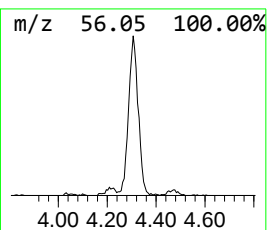
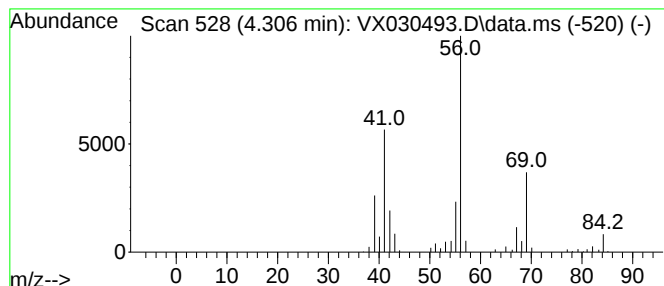
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Cyclic4.306 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	13.14 ug/L	188289	1,4-Difluorobenzene	6.769

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2		Cyclopentane, methyl-	84	C6H12	000096-37-7	90
3		Cyclopentane, methyl-	84	C6H12	000096-37-7	78
4		Cyclopentane, methyl-	84	C6H12	000096-37-7	72
5		Cyclobutane, ethyl-	84	C6H12	004806-61-5	72



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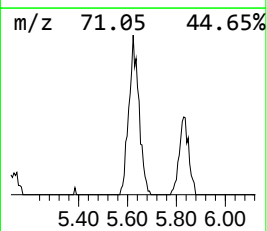
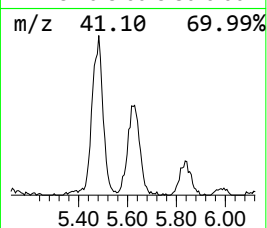
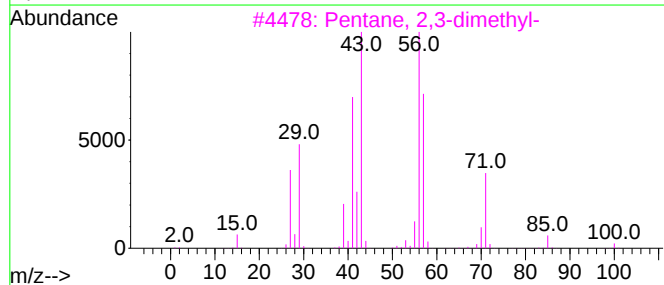
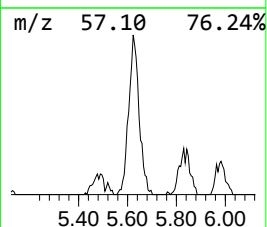
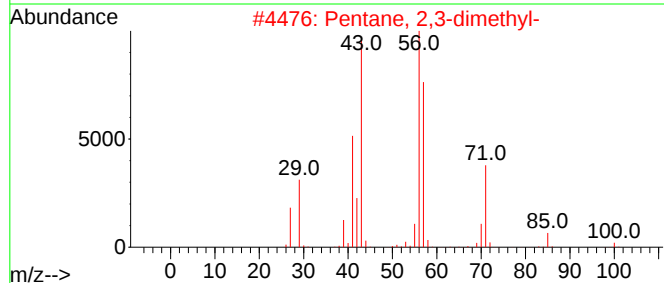
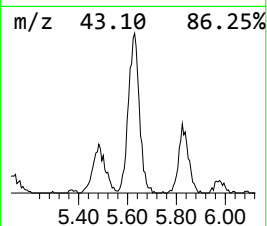
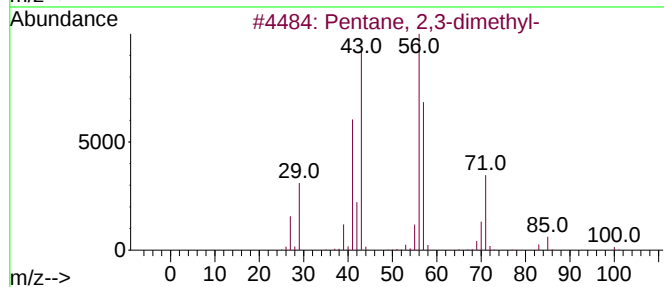
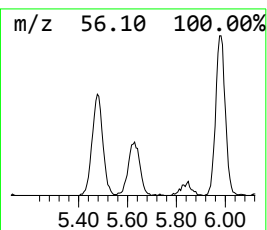
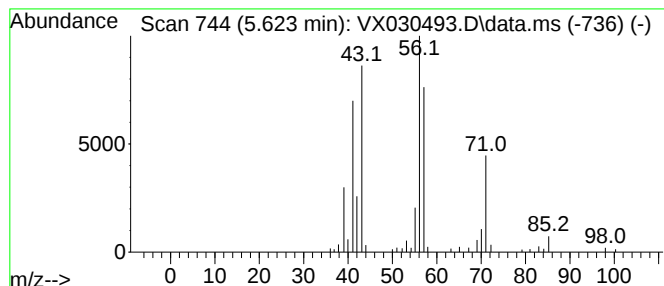
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.623	7.71 ug/L	110519	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	90
2			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	90
3			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	72
4			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	64
5			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080622\
Data File : VX030493.D
Acq On : 07 Aug 2022 03:16
Operator : JC/MD
Sample : N4021-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
F5D67

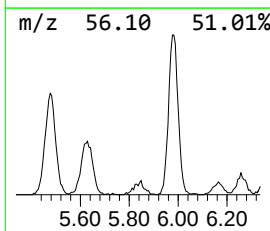
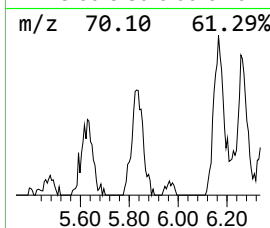
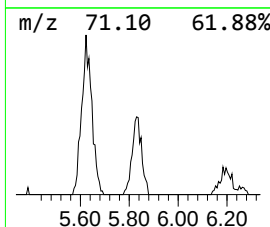
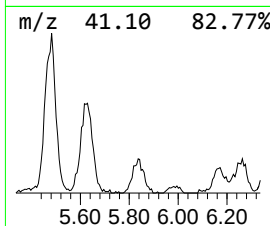
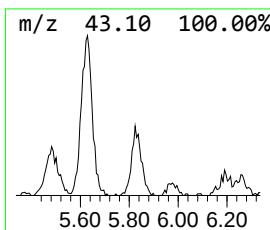
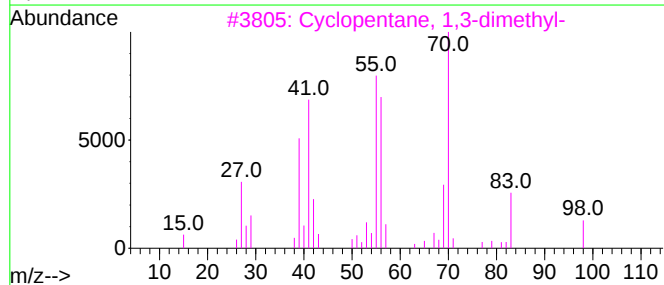
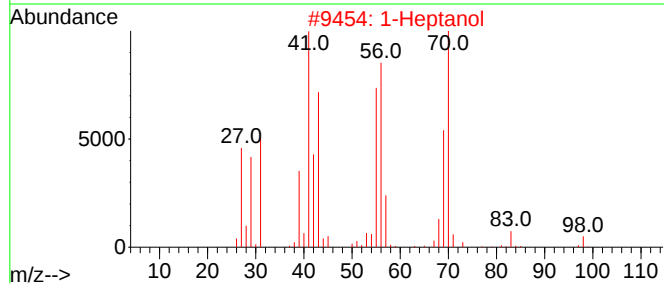
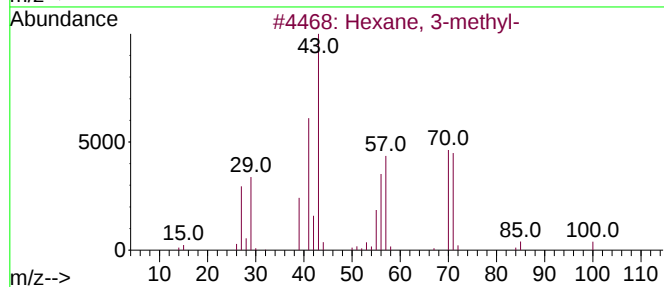
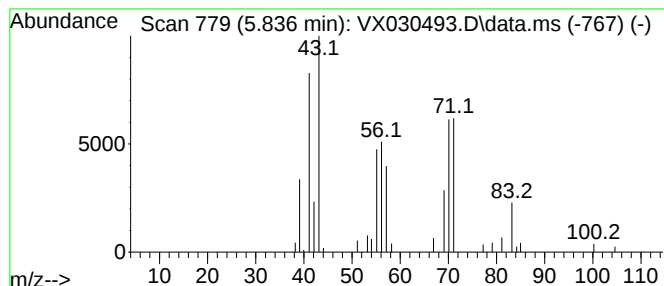
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.836	3.21 ug/L	46001	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	53
2			1-Heptanol	116	C7H16O	000111-70-6	47
3			Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	47
4			Oxirane, (3-methylbutyl)-	114	C7H14O	053229-41-7	47
5			Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080622\
Data File : VX030493.D
Acq On : 07 Aug 2022 03:16
Operator : JC/MD
Sample : N4021-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
F5D67

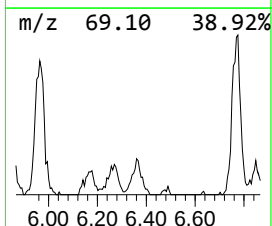
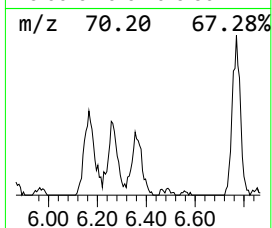
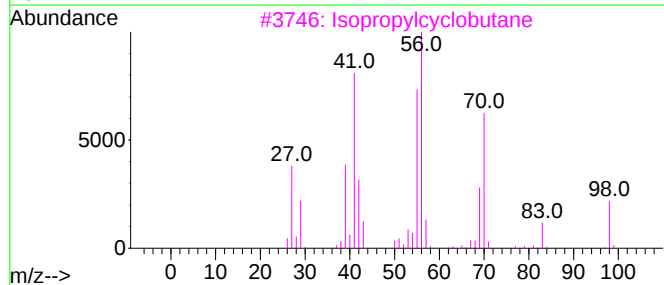
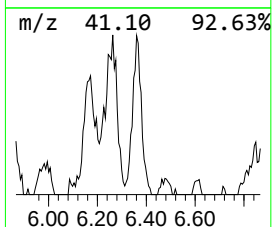
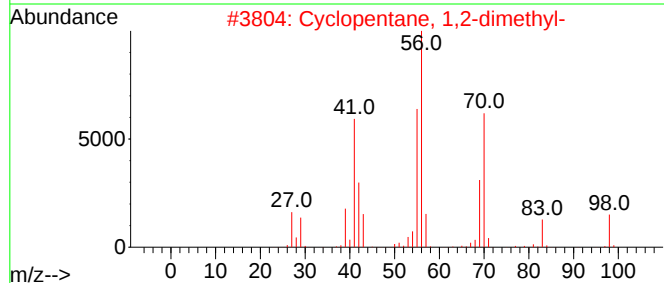
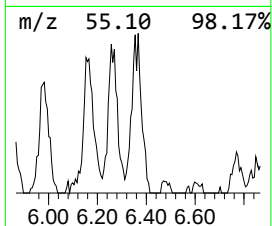
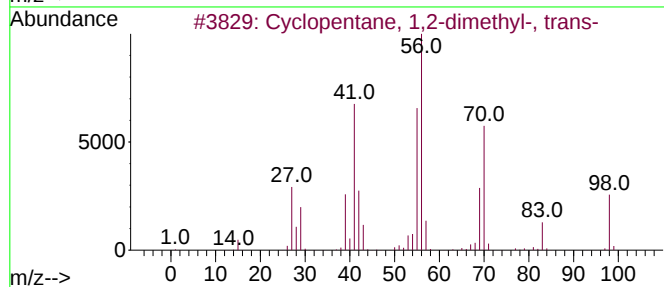
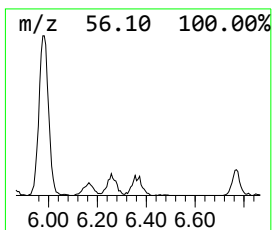
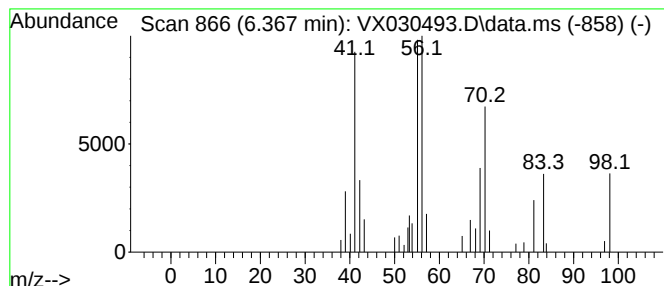
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Quant Title : VOC Analysis

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

Peak Number 5 (DEL) Alkane: Cyclic6.367 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.367	2.67 ug/L	38261	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	81
2			Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	72
3			Isopropylcyclobutane	98	C7H14	000872-56-0	64
4			Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	64
5			1-Pentene, 3-ethyl-	98	C7H14	004038-04-4	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080622\
Data File : VX030493.D
Acq On : 07 Aug 2022 03:16
Operator : JC/MD
Sample : N4021-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
F5D67

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.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...	2.825	3.1	ug/L	44744	1	6.769	716311	50.0
(DEL) Alkane: C...	4.306	13.1	ug/L	188289	1	6.769	716311	50.0
(DEL) Alkane: S...	5.623	7.7	ug/L	110519	1	6.769	716311	50.0
(DEL) Alkane: S...	5.836	3.2	ug/L	46001	1	6.769	716311	50.0
(DEL) Alkane: C...	6.367	2.7	ug/L	38261	1	6.769	716311	50.0