

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080522\
 Data File : VX030444.D
 Acq On : 05 Aug 2022 21:38
 Operator : JC/MD
 Sample : N4066-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 F5D93

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: VX030444.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	59	rVB	2381498	2595267	22.64%	9.705%
2	1.666	91	95	104	rVB2	103477	149202	1.30%	0.558%
3	1.746	104	108	117	rVB	66944	90785	0.79%	0.339%
4	1.953	138	142	151	rVB2	19652	30061	0.26%	0.112%
5	2.203	181	183	185	rBV3	1331	1365	0.01%	0.005%
6	2.307	194	200	211	rVB2	225977	392079	3.42%	1.466%
7	2.575	241	244	247	rVB2	392	483	0.00%	0.002%
8	2.624	250	252	254	rBV	486	428	0.00%	0.002%
9	2.782	271	278	281	rBV2	17049	37192	0.32%	0.139%
10	2.825	281	285	289	rVV2	26146	42662	0.37%	0.160%
11	2.989	307	312	314	rBV3	1744	3305	0.03%	0.012%
12	3.099	321	330	348	rBV3	302820	723079	6.31%	2.704%
13	3.319	365	366	367	rBV	668	359	0.00%	0.001%
14	3.367	372	374	376	rVB2	616	526	0.00%	0.002%
15	3.447	379	387	393	rBV6	1593	3643	0.03%	0.014%
16	3.532	398	401	404	rVB2	631	539	0.00%	0.002%
17	3.569	404	407	411	rBV2	777	1185	0.01%	0.004%
18	3.636	416	418	422	rBV2	405	770	0.01%	0.003%
19	3.739	432	435	436	rBV2	763	757	0.01%	0.003%
20	3.788	442	443	445	rBV	398	340	0.00%	0.001%
21	3.904	459	462	463	rBV	281	336	0.00%	0.001%
22	4.105	492	495	498	rBV2	448	631	0.01%	0.002%
23	4.160	503	504	507	rVB	560	387	0.00%	0.001%
24	4.196	507	510	512	rBV2	895	1113	0.01%	0.004%
25	4.306	519	528	542	rVB2	40034	112594	0.98%	0.421%
26	4.410	542	545	546	rBV	522	659	0.01%	0.002%
27	4.495	546	559	581	rBV	4239772	11463600	100.00%	42.866%
28	4.824	612	613	617	rBV2	842	930	0.01%	0.003%
29	5.068	641	653	668	rBV	143076	449534	3.92%	1.681%
30	5.391	703	706	708	rVV2	586	718	0.01%	0.003%
31	5.471	709	719	732	rVV2	26483	83558	0.73%	0.312%
32	5.782	767	770	771	rBV2	453	515	0.00%	0.002%
33	5.855	773	782	790	rBV6	3480	10689	0.09%	0.040%
34	5.977	790	802	809	rBV2	372522	1100224	9.60%	4.114%
35	6.355	858	864	876	rVB6	6127	17434	0.15%	0.065%
36	6.440	876	878	883	rVB2	547	908	0.01%	0.003%

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Integrator: RTE

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 Title : VOC Analysis

37	6.483	883	885	886	rBV	449	387	0.00%	0.001%
38	6.769	922	932	946	rVV	288456	678982	5.92%	2.539%
39	6.964	962	964	966	rVB2	532	474	0.00%	0.002%
40	7.001	966	970	971	rBV2	409	408	0.00%	0.002%
41	7.129	982	991	1010	rBV	1411999	3075115	26.83%	11.499%
42	7.312	1013	1021	1029	rBV	230000	520047	4.54%	1.945%
43	7.574	1062	1064	1067	rVB3	766	604	0.01%	0.002%
44	7.659	1069	1078	1084	rVB6	2459	5324	0.05%	0.020%
45	7.745	1090	1092	1094	rBV	357	372	0.00%	0.001%
46	7.873	1110	1113	1117	rVB4	702	926	0.01%	0.003%
47	7.909	1117	1119	1121	rVB	548	361	0.00%	0.001%
48	7.958	1125	1127	1128	rVB2	551	333	0.00%	0.001%
49	8.080	1145	1147	1148	rVB	610	346	0.00%	0.001%
50	8.330	1181	1188	1198	rBV	156724	248622	2.17%	0.930%
51	8.440	1202	1206	1209	rBV3	857	1647	0.01%	0.006%
52	8.653	1234	1241	1250	rBV	552508	852861	7.44%	3.189%
53	8.897	1280	1281	1283	rBV	616	461	0.00%	0.002%
54	8.952	1285	1290	1300	rVV	108031	162878	1.42%	0.609%
55	9.147	1318	1322	1323	rBV3	669	702	0.01%	0.003%
56	9.189	1327	1329	1331	rBV	798	802	0.01%	0.003%
57	9.214	1331	1333	1336	rVB2	439	339	0.00%	0.001%
58	9.275	1337	1343	1354	rVB	280563	416947	3.64%	1.559%
59	9.391	1356	1362	1375	rBV	473641	679973	5.93%	2.543%
60	9.738	1415	1419	1422	rBV4	698	1373	0.01%	0.005%
61	9.866	1435	1440	1442	rBV3	408	555	0.00%	0.002%
62	9.891	1442	1444	1446	rBV	358	418	0.00%	0.002%
63	10.055	1466	1471	1479	rBV	555941	764737	6.67%	2.860%
64	10.165	1488	1489	1492	rVB2	646	328	0.00%	0.001%
65	10.354	1519	1520	1522	rBV2	439	408	0.00%	0.002%
66	10.811	1590	1595	1597	rBV	539	855	0.01%	0.003%
67	10.836	1597	1599	1602	rVB2	475	564	0.00%	0.002%
68	10.866	1602	1604	1606	rBV	594	420	0.00%	0.002%
69	11.025	1627	1630	1633	rBV2	695	874	0.01%	0.003%
70	11.092	1638	1641	1644	rVB3	517	608	0.01%	0.002%
71	11.146	1648	1650	1652	rBV	475	432	0.00%	0.002%
72	11.195	1652	1658	1666	rBV	418167	531408	4.64%	1.987%
73	11.342	1680	1682	1686	rVB3	437	629	0.01%	0.002%
74	11.384	1686	1689	1690	rBV2	487	352	0.00%	0.001%
75	11.433	1693	1697	1698	rBV2	464	620	0.01%	0.002%
76	11.689	1737	1739	1740	rBV	785	347	0.00%	0.001%

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77	11.921	1776	1777	1779	rBV2	392	407	0.00%	0.002%
78	12.024	1789	1794	1801	rBV	613976	715909	6.25%	2.677%
79	12.323	1837	1843	1849	rBV	598044	743716	6.49%	2.781%
80	12.457	1863	1865	1867	rBV	449	457	0.00%	0.002%
81	12.628	1891	1893	1895	rBV2	390	336	0.00%	0.001%
82	12.750	1911	1913	1915	rBV	481	345	0.00%	0.001%
83	12.774	1915	1917	1919	rVV2	449	380	0.00%	0.001%
84	13.347	2009	2011	2013	rVV2	486	505	0.00%	0.002%
85	13.506	2035	2037	2038	rBV	423	421	0.00%	0.002%
86	13.518	2038	2039	2041	rVB	705	370	0.00%	0.001%
87	13.664	2059	2063	2064	rBV	486	436	0.00%	0.002%
88	14.073	2128	2130	2132	rVB	529	376	0.00%	0.001%
89	14.201	2150	2151	2154	rBV2	552	559	0.00%	0.002%
90	14.347	2172	2175	2177	rBV	450	417	0.00%	0.002%
91	14.634	2220	2222	2225	rVB2	483	512	0.00%	0.002%
92	14.658	2225	2226	2228	rBV2	737	615	0.01%	0.002%
93	15.121	2300	2302	2304	rBV2	786	623	0.01%	0.002%
94	15.377	2343	2344	2348	rBV3	586	726	0.01%	0.003%
95	15.451	2353	2356	2358	rBV3	572	782	0.01%	0.003%
96	15.755	2405	2406	2407	rVB	944	346	0.00%	0.001%
97	15.890	2427	2428	2430	rBV	694	655	0.01%	0.002%
98	15.938	2434	2436	2437	rVB2	772	414	0.00%	0.002%
99	15.957	2437	2439	2443	rBV2	682	1128	0.01%	0.004%
100	16.377	2506	2508	2511	rBV2	842	695	0.01%	0.003%

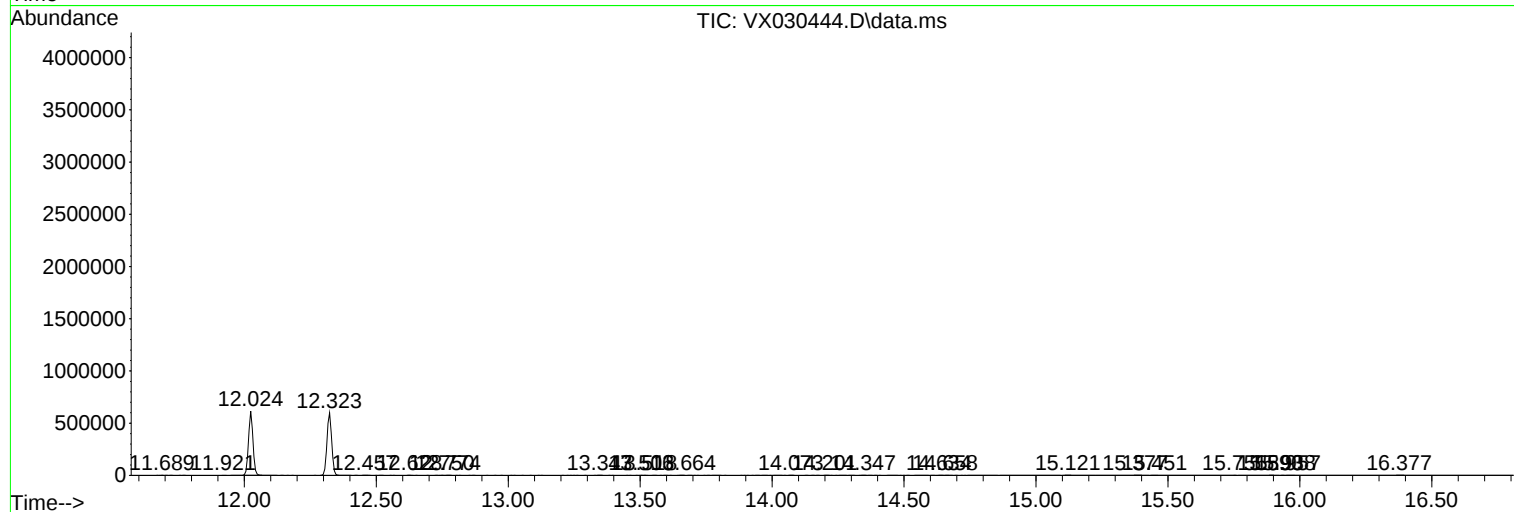
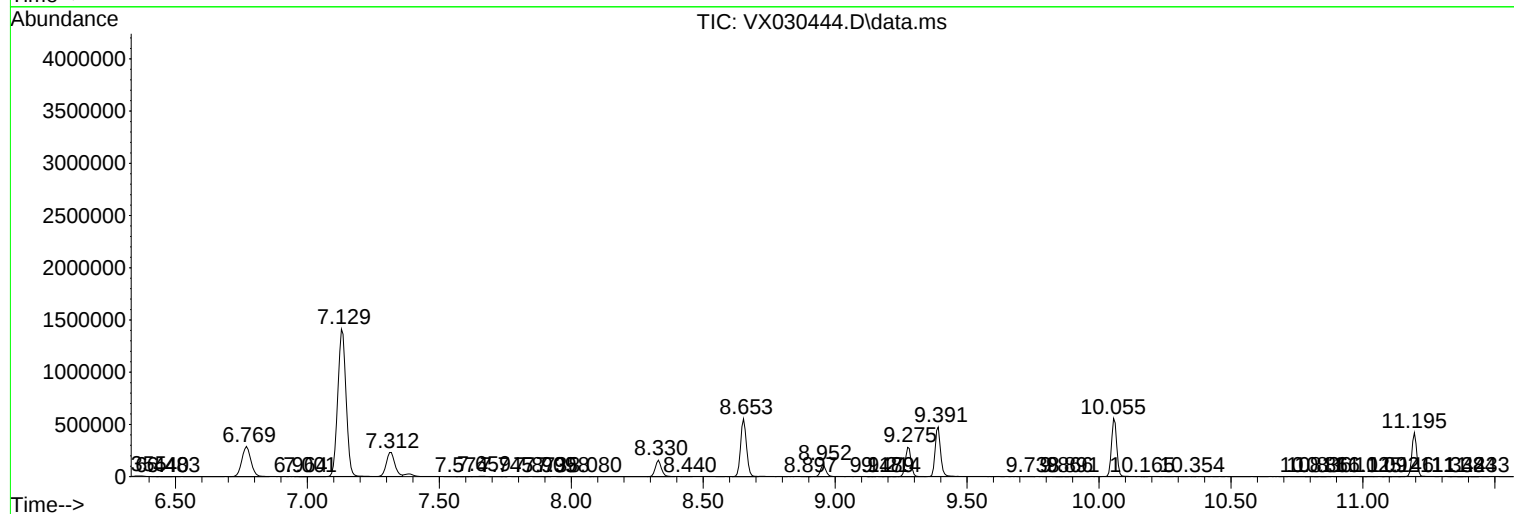
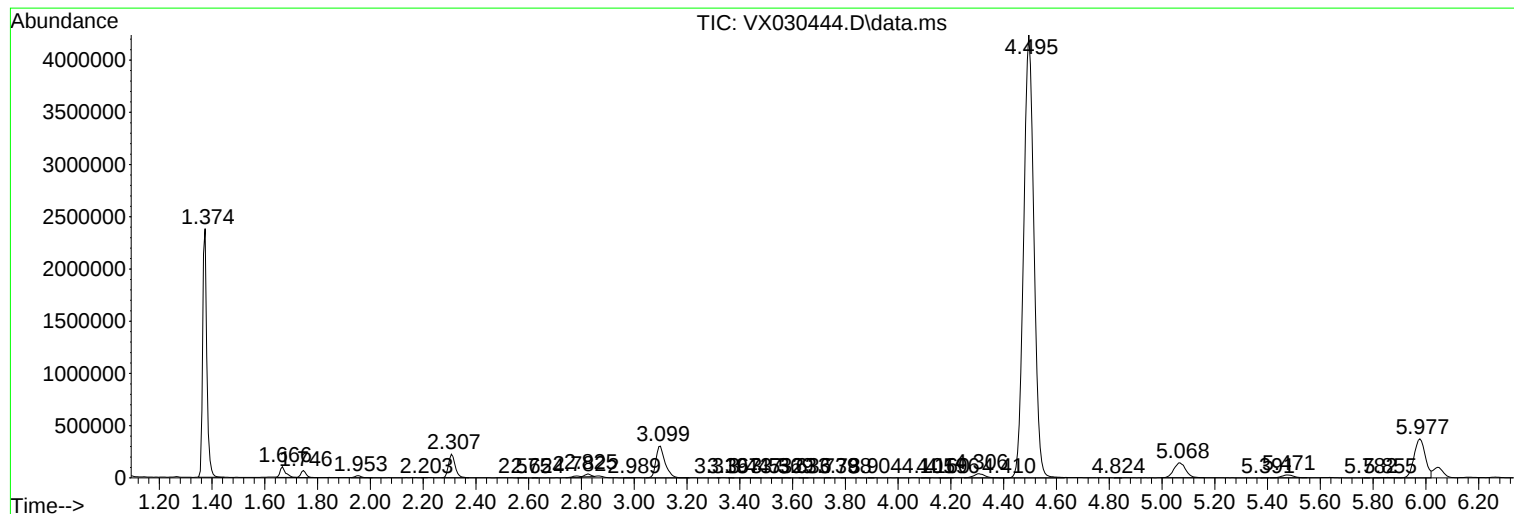
Sum of corrected areas: 26742826

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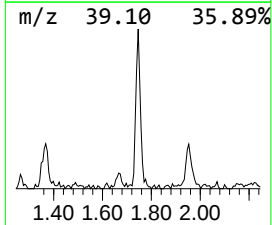
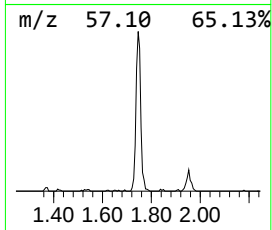
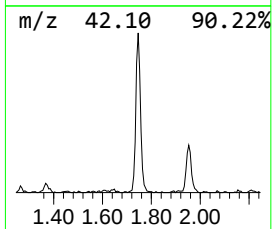
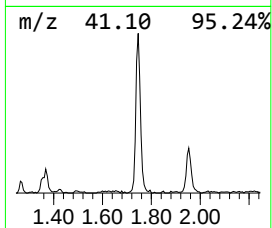
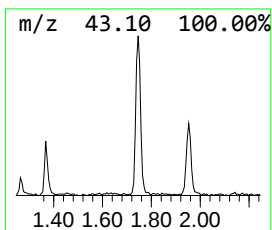
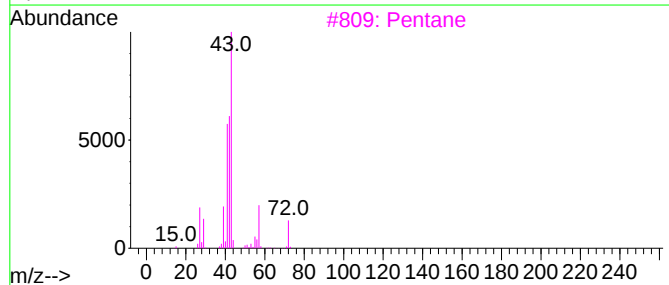
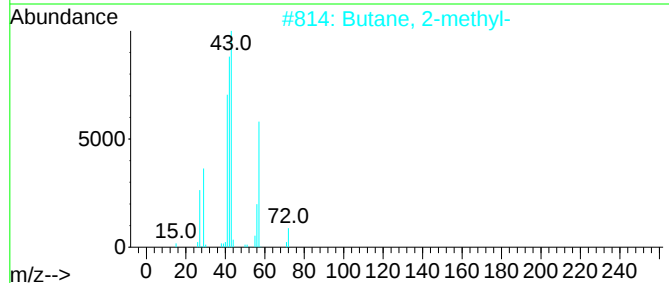
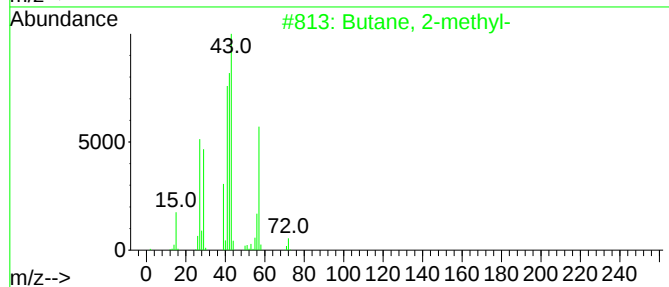
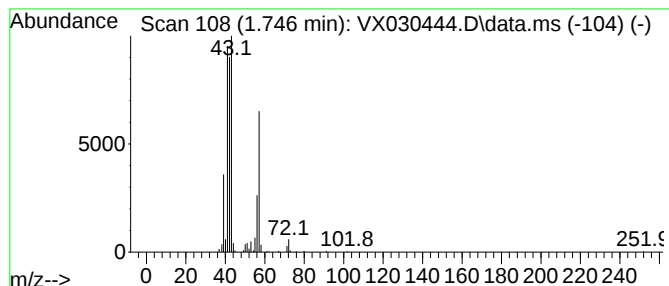
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.746	6.69 ug/L	90785	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	86
2			Butane, 2-methyl-	72	C5H12	000078-78-4	64
3			Pentane	72	C5H12	000109-66-0	36
4			2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	12
5			1-Butene	56	C4H8	000106-98-9	10



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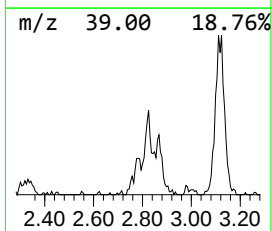
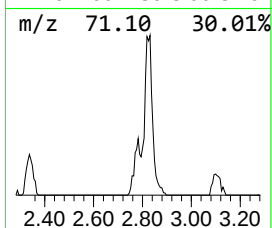
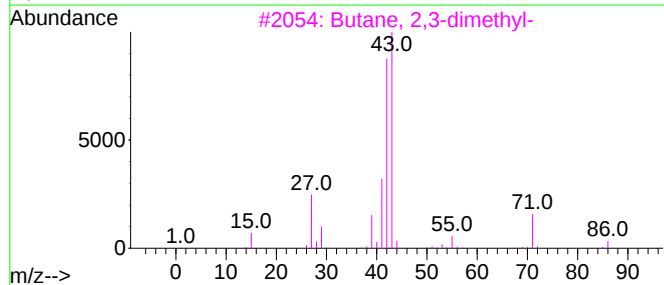
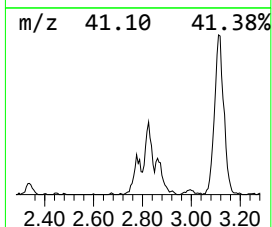
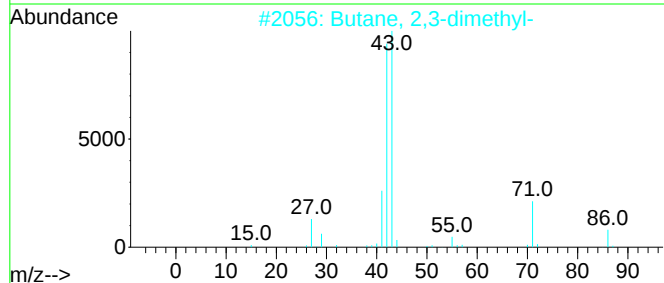
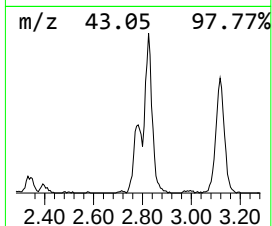
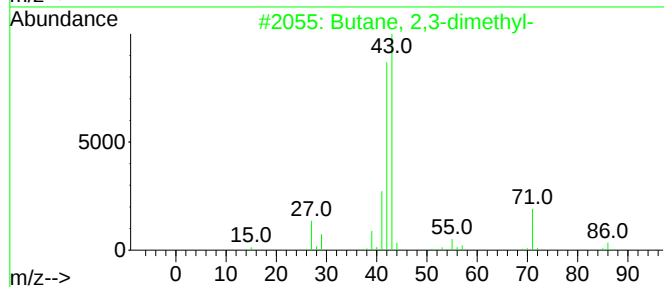
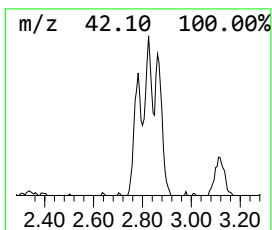
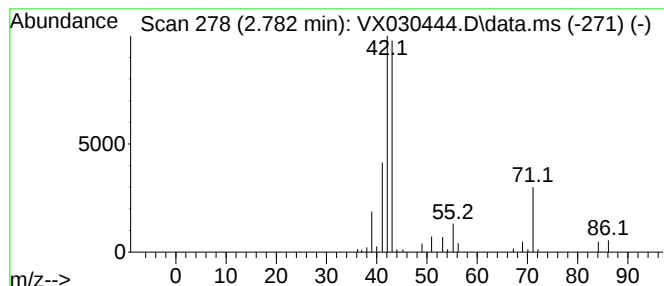
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	2.74 ug/L	37192	1,4-Difluorobenzene	6.769

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	80
2		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	64
3		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	59
4		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	47
5		Pentane, 2-methyl-	86	C6H14	000107-83-5	38



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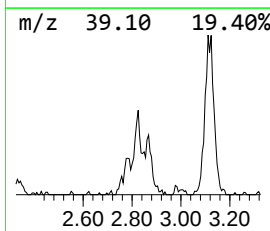
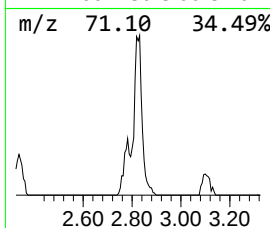
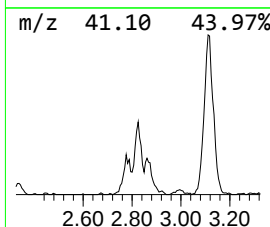
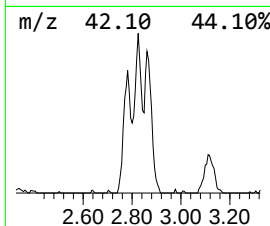
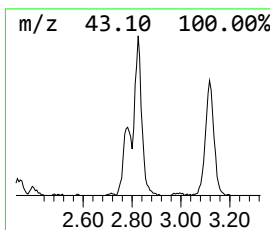
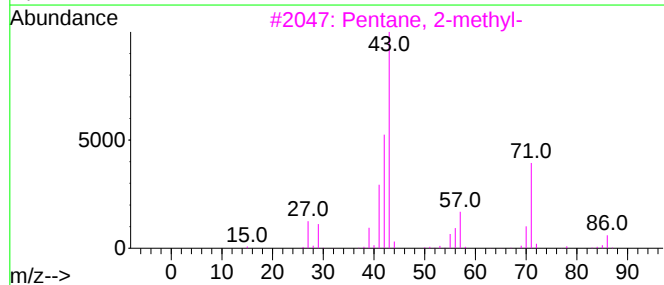
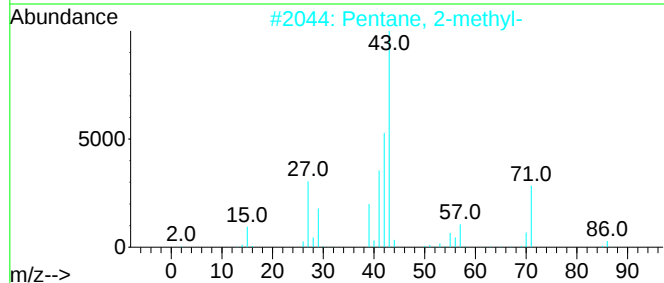
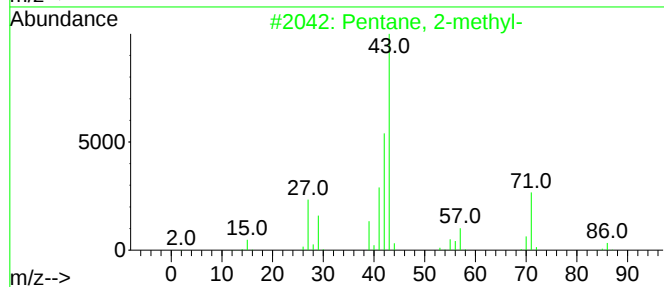
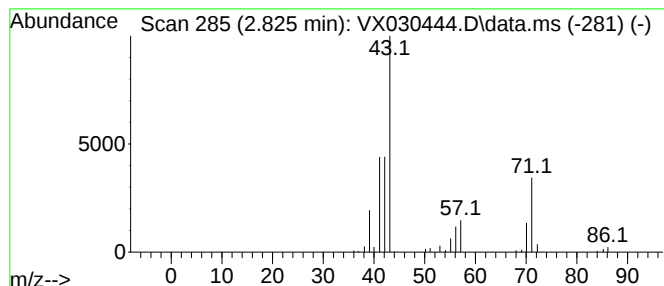
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.825	3.14 ug/L	42662	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-methyl-	86	C6H14	000107-83-5	86
3			Pentane, 2-methyl-	86	C6H14	000107-83-5	78
4			Pentane, 2-methyl-	86	C6H14	000107-83-5	64
5			Pentane, 2-methyl-	86	C6H14	000107-83-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080522\
Data File : VX030444.D
Acq On : 05 Aug 2022 21:38
Operator : JC/MD
Sample : N4066-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 32 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
F5D93

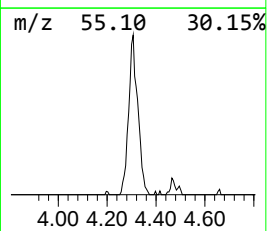
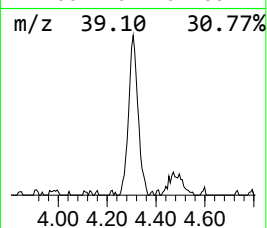
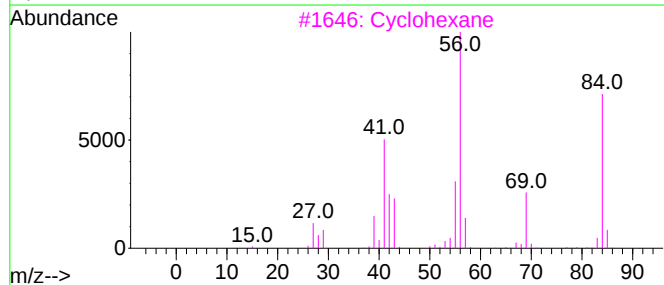
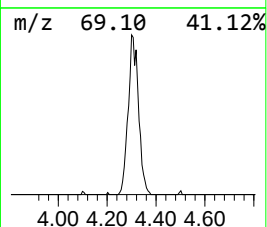
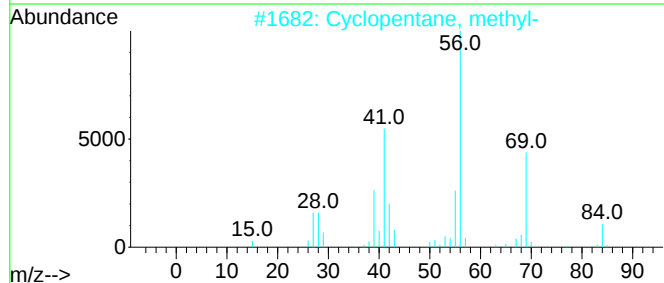
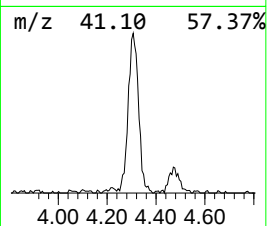
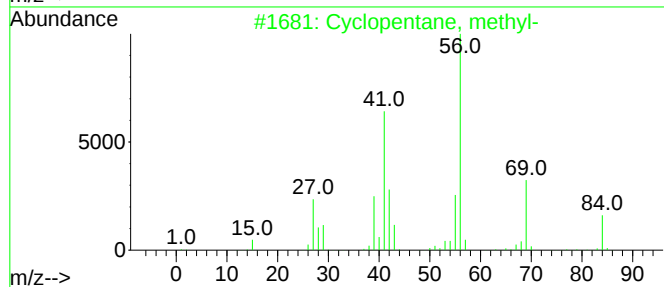
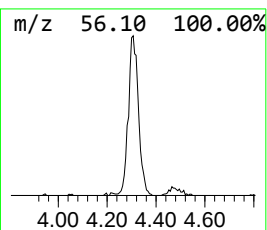
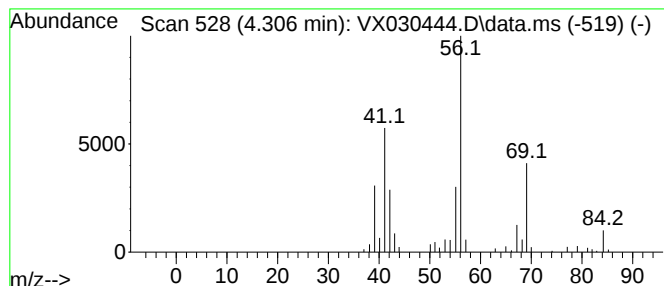
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Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Cyclic4.306 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	8.29 ug/L	112594	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	87
2			Cyclopentane, methyl-	84	C6H12	000096-37-7	83
3			Cyclohexane	84	C6H12	000110-82-7	78
4			Cyclopentane, methyl-	84	C6H12	000096-37-7	78
5			Cyclohexane	84	C6H12	000110-82-7	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080522\
Data File : VX030444.D
Acq On : 05 Aug 2022 21:38
Operator : JC/MD
Sample : N4066-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 32 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
F5D93

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...	1.746	6.7	ug/L	90785	1	6.769	678982	50.0
(DEL) Alkane: S...	2.782	2.7	ug/L	37192	1	6.769	678982	50.0
(DEL) Alkane: S...	2.825	3.1	ug/L	42662	1	6.769	678982	50.0
(DEL) Alkane: C...	4.306	8.3	ug/L	112594	1	6.769	678982	50.0