

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122723\
 Data File : VX039497.D
 Acq On : 27 Dec 2023 15:21
 Operator : JC/MD
 Sample : 05989-02DL 4X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 F7A61DL

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\SFAMXML120523WMA.M

Title : VOC Analysis

Signal : TIC: VX039497.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	22	27	40	rBV2	6580	18354	2.72%	0.260%
2	1.368	43	46	57	rBV	62129	76376	11.32%	1.081%
3	1.453	57	60	64	rVV	3838	4558	0.68%	0.064%
4	1.648	88	92	106	rVB	46067	73965	10.96%	1.047%
5	2.300	193	199	207	rBV	130988	203382	30.14%	2.878%
6	2.386	208	213	217	rBV	25587	47457	7.03%	0.671%
7	2.581	237	245	253	rVB2	7921	19104	2.83%	0.270%
8	2.709	262	266	274	rVB	4912	8743	1.30%	0.124%
9	2.788	274	279	286	rVB	2422	3826	0.57%	0.054%
10	2.947	297	305	318	rVB	8751	20794	3.08%	0.294%
11	3.044	318	321	322	rVB2	355	339	0.05%	0.005%
12	3.422	381	383	387	rVB	266	303	0.04%	0.004%
13	3.916	462	464	468	rVB3	499	504	0.07%	0.007%
14	4.020	480	481	486	rVB	382	335	0.05%	0.005%
15	4.062	486	488	492	rBV2	316	433	0.06%	0.006%
16	4.184	505	508	512	rBV2	210	363	0.05%	0.005%
17	4.276	521	523	526	rVB	338	271	0.04%	0.004%
18	4.355	533	536	540	rBV3	362	435	0.06%	0.006%
19	4.465	545	554	563	rBV	79642	244306	36.21%	3.457%
20	4.562	564	570	593	rVB	80529	242553	35.95%	3.432%
21	4.843	614	616	619	rVB2	468	392	0.06%	0.006%
22	5.056	638	651	666	rBV3	113671	370045	54.84%	5.236%
23	5.538	728	730	732	rBV3	301	327	0.05%	0.005%
24	5.708	754	758	759	rBV	207	311	0.05%	0.004%
25	5.824	775	777	780	rVB	228	256	0.04%	0.004%
26	5.855	780	782	784	rBV2	292	312	0.05%	0.004%
27	5.970	789	801	814	rBV2	228665	674758	100.00%	9.547%
28	6.172	827	834	836	rBV5	959	2021	0.30%	0.029%
29	6.367	862	866	869	rVV3	469	782	0.12%	0.011%
30	6.659	908	914	916	rBV2	332	628	0.09%	0.009%
31	6.763	921	931	949	rBV	196484	477409	70.75%	6.755%
32	6.952	961	962	967	rVB2	382	332	0.05%	0.005%
33	7.080	981	983	988	rVB	247	317	0.05%	0.004%
34	7.238	1002	1009	1013	rBV2	7105	15545	2.30%	0.220%
35	7.306	1013	1020	1033	rVB	145363	319538	47.36%	4.521%
36	7.464	1041	1046	1060	rVB2	14597	34233	5.07%	0.484%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
 Title : VOC Analysis

37	7.580	1063	1065	1066	rBV2	357	341	0.05%	0.005%
38	7.757	1092	1094	1096	rVB	324	253	0.04%	0.004%
39	7.787	1096	1099	1102	rBV2	241	327	0.05%	0.005%
40	7.830	1102	1106	1108	rBV2	289	298	0.04%	0.004%
41	7.927	1114	1122	1125	rBV4	3782	8038	1.19%	0.114%
42	8.324	1181	1187	1201	rBV	88935	153425	22.74%	2.171%
43	8.500	1214	1216	1218	rVV	501	278	0.04%	0.004%
44	8.586	1224	1230	1234	rBV	3768	6885	1.02%	0.097%
45	8.647	1234	1240	1251	rBV	319237	509854	75.56%	7.214%
46	8.897	1279	1281	1285	rBV2	351	361	0.05%	0.005%
47	8.952	1285	1290	1303	rBV	66413	102957	15.26%	1.457%
48	9.269	1335	1342	1348	rBV7	1267	3175	0.47%	0.045%
49	9.342	1348	1354	1356	rBV5	3456	4837	0.72%	0.068%
50	9.384	1356	1361	1381	rVB	374529	555529	82.33%	7.860%
51	9.720	1415	1416	1422	rVB3	814	983	0.15%	0.014%
52	10.055	1465	1471	1481	rBV	423061	579326	85.86%	8.197%
53	10.512	1543	1546	1548	rBV2	356	366	0.05%	0.005%
54	10.585	1552	1558	1565	rBV3	3017	6015	0.89%	0.085%
55	10.768	1579	1588	1601	rBV	54366	76381	11.32%	1.081%
56	10.884	1602	1607	1616	rBV	12094	21242	3.15%	0.301%
57	11.006	1625	1627	1631	rVB3	473	351	0.05%	0.005%
58	11.091	1637	1641	1644	rVB3	1247	1577	0.23%	0.022%
59	11.195	1652	1658	1665	rBV	295522	394731	58.50%	5.585%
60	11.378	1686	1688	1689	rBV2	303	258	0.04%	0.004%
61	11.433	1694	1697	1699	rBV4	917	1018	0.15%	0.014%
62	11.597	1721	1724	1725	rBV3	686	726	0.11%	0.010%
63	11.689	1735	1739	1741	rBV2	1163	1821	0.27%	0.026%
64	11.756	1746	1750	1760	rBV	345221	423353	62.74%	5.990%
65	11.847	1760	1765	1771	rBV2	111156	173010	25.64%	2.448%
66	12.024	1789	1794	1805	rVB	442167	589923	87.43%	8.347%
67	12.146	1811	1814	1819	rVB5	2299	3218	0.48%	0.046%
68	12.225	1823	1827	1833	rVV4	3052	5709	0.85%	0.081%
69	12.317	1837	1842	1853	rVB	385809	509560	75.52%	7.210%
70	12.506	1871	1873	1877	rBV4	532	727	0.11%	0.010%
71	12.561	1879	1882	1886	rBV3	1008	1446	0.21%	0.020%
72	12.664	1897	1899	1900	rBV2	427	305	0.05%	0.004%
73	12.695	1900	1904	1909	rVB5	1394	2380	0.35%	0.034%
74	12.768	1909	1916	1919	rBV2	5084	7113	1.05%	0.101%
75	12.859	1929	1931	1934	rVB3	1080	1049	0.16%	0.015%
76	13.006	1953	1955	1957	rBV2	308	269	0.04%	0.004%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120523WMA.M
 Title : VOC Analysis

77	13.030	1957	1959	1962	rBV	199	254	0.04%	0.004%
78	13.146	1974	1978	1979	rBV2	219	288	0.04%	0.004%
79	13.170	1979	1982	1985	rBV3	787	1105	0.16%	0.016%
80	13.243	1990	1994	1999	rVB3	227	448	0.07%	0.006%
81	13.341	2006	2010	2014	rBV4	214	377	0.06%	0.005%
82	13.439	2020	2026	2031	rBV2	548	1142	0.17%	0.016%
83	13.518	2034	2039	2047	rBV	32196	42448	6.29%	0.601%
84	13.682	2063	2066	2067	rBV	333	381	0.06%	0.005%
85	13.780	2078	2082	2085	rVB	1324	1394	0.21%	0.020%
86	14.121	2137	2138	2142	rBV2	400	393	0.06%	0.006%
87	14.280	2161	2164	2165	rBV	264	254	0.04%	0.004%
88	14.304	2165	2168	2172	rVV3	1105	1229	0.18%	0.017%
89	14.371	2176	2179	2183	rVV3	399	575	0.09%	0.008%
90	14.554	2206	2209	2212	rVB	258	269	0.04%	0.004%
91	14.640	2220	2223	2227	rVB3	463	607	0.09%	0.009%
92	15.042	2287	2289	2291	rBV2	416	428	0.06%	0.006%
93	15.121	2300	2302	2304	rBV	261	297	0.04%	0.004%
94	15.237	2318	2321	2324	rBV2	314	456	0.07%	0.006%
95	15.353	2336	2340	2342	rBV4	331	411	0.06%	0.006%
96	15.505	2362	2365	2367	rBV2	352	465	0.07%	0.007%
97	15.639	2386	2387	2390	rVV2	265	256	0.04%	0.004%
98	15.767	2404	2408	2410	rBV2	312	402	0.06%	0.006%
99	15.798	2410	2413	2416	rVV2	325	382	0.06%	0.005%
100	16.072	2456	2458	2461	rBV3	406	458	0.07%	0.006%

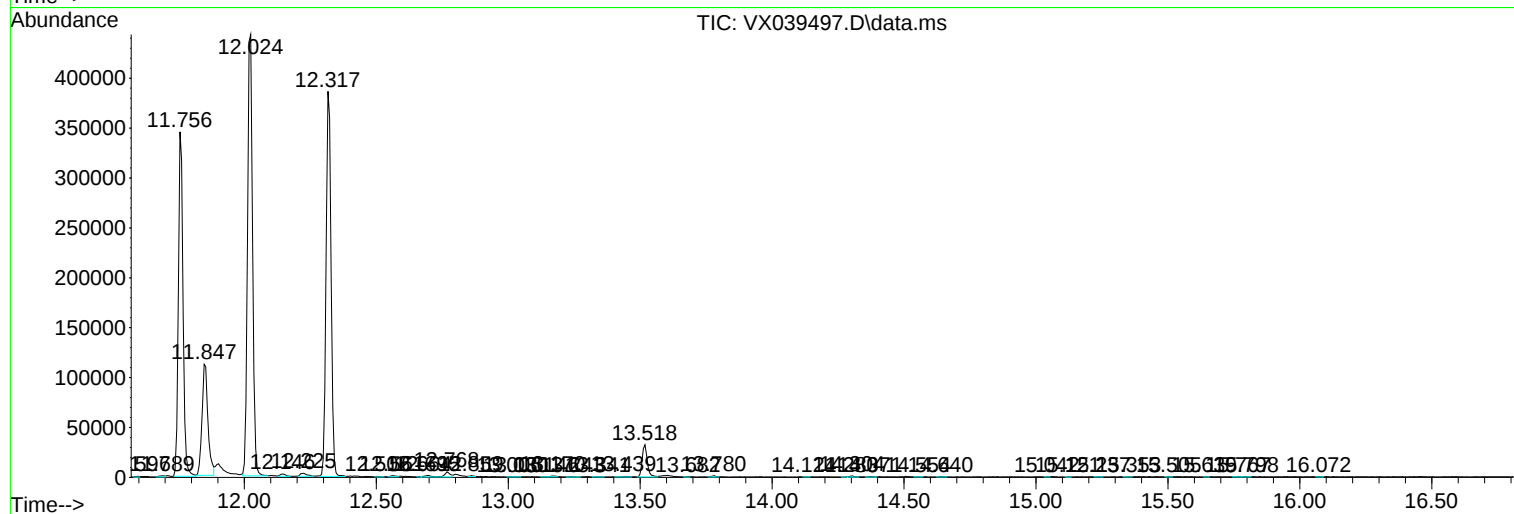
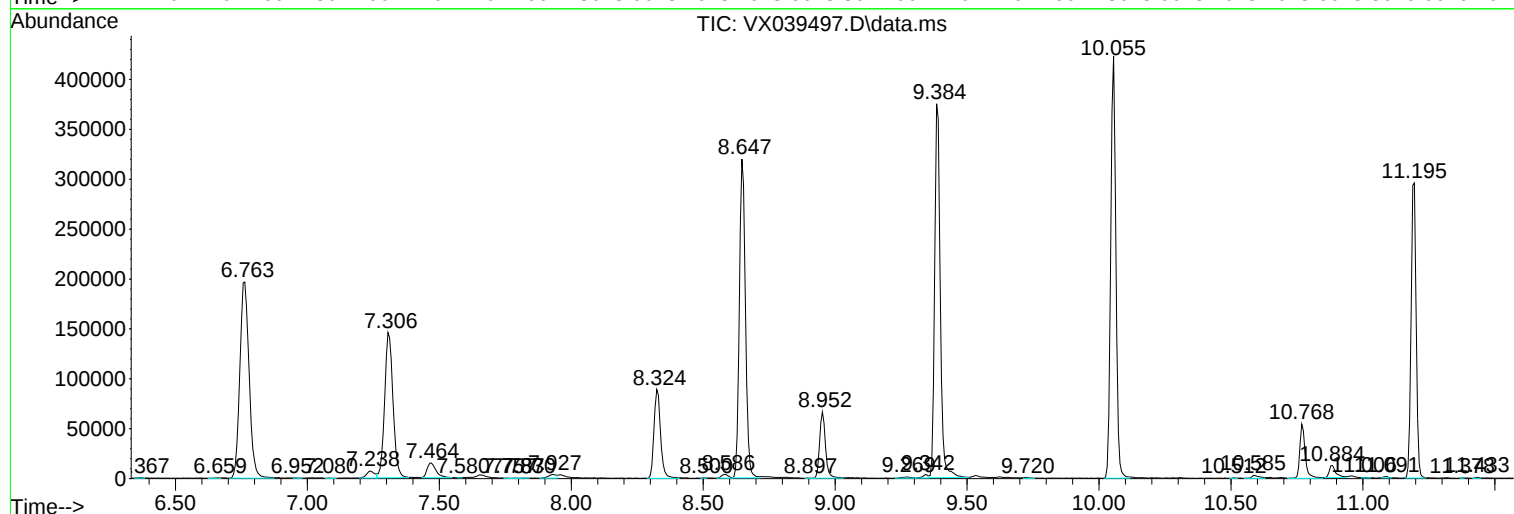
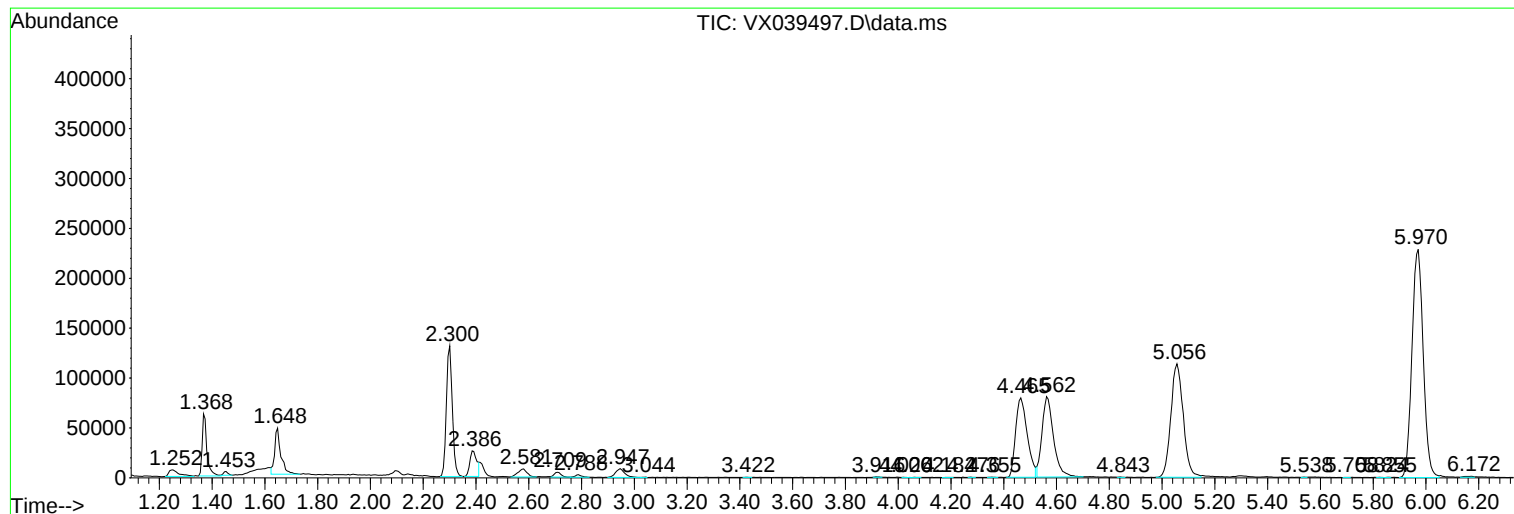
Sum of corrected areas: 7067741

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Instrument :
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ClientSampleId :
F7A61DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.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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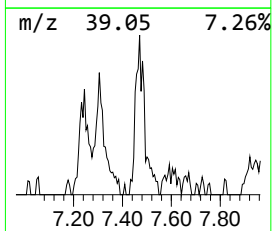
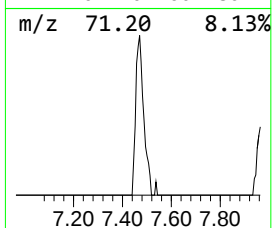
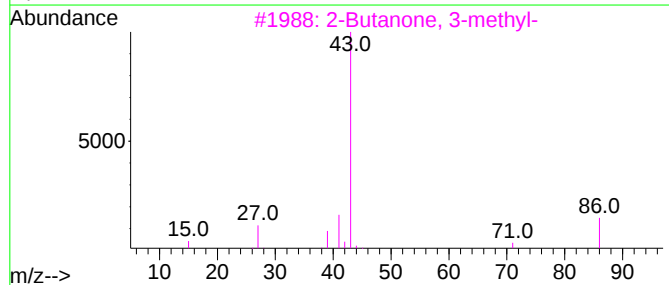
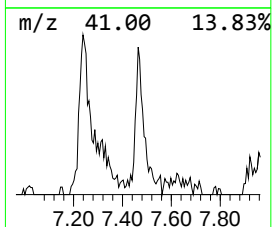
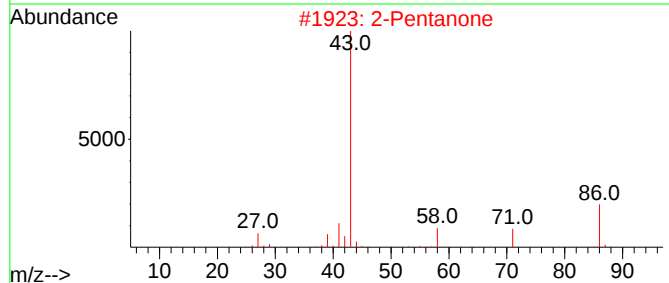
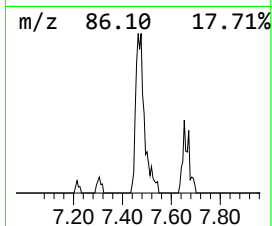
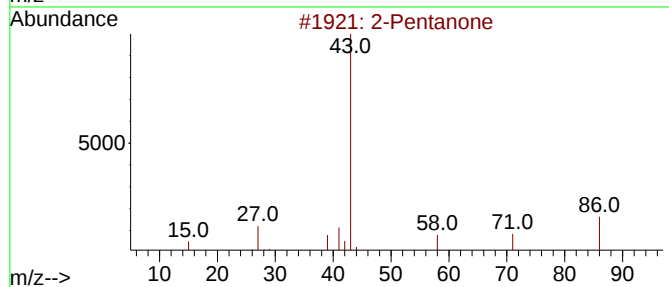
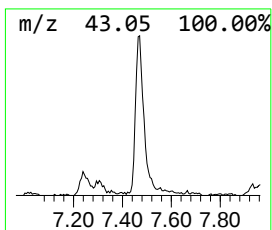
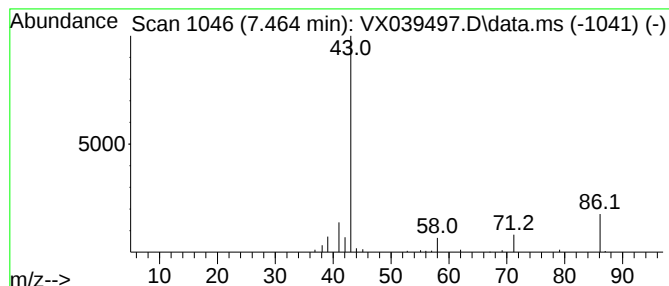
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 2-Pentanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.464	3.59 ug/L	34233	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone			86	C5H10O	000107-87-9	59
2	2-Pentanone			86	C5H10O	000107-87-9	53
3	2-Butanone, 3-methyl-			86	C5H10O	000563-80-4	50
4	2,3-Butanedione			86	C4H6O2	000431-03-8	40
5	2-Butanone, 3-methyl-			86	C5H10O	000563-80-4	40



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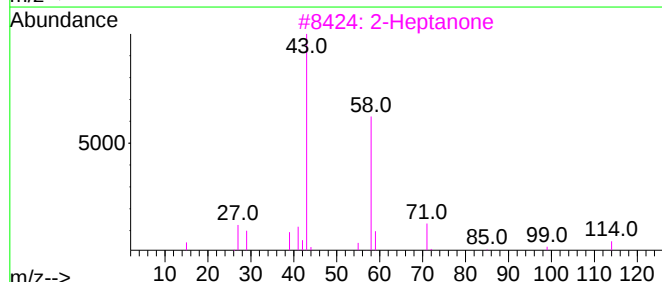
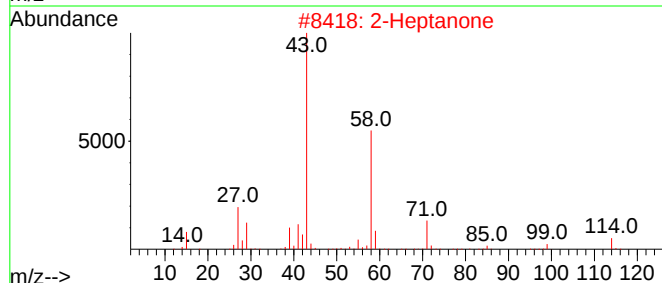
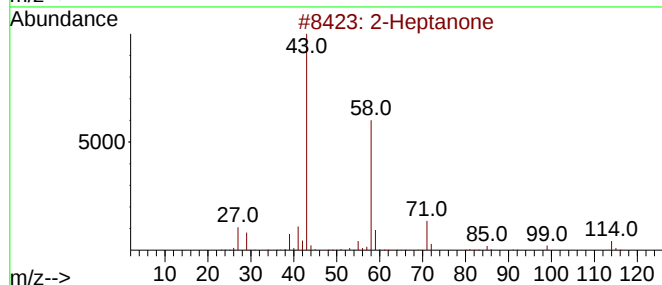
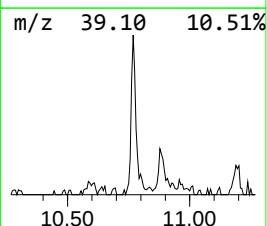
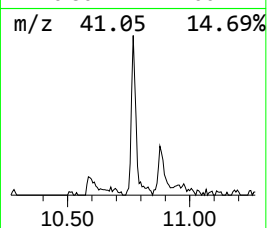
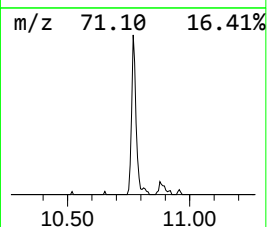
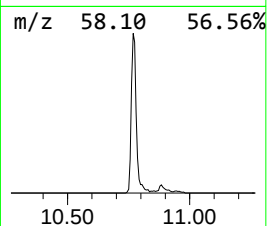
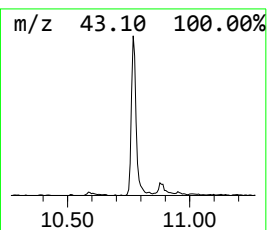
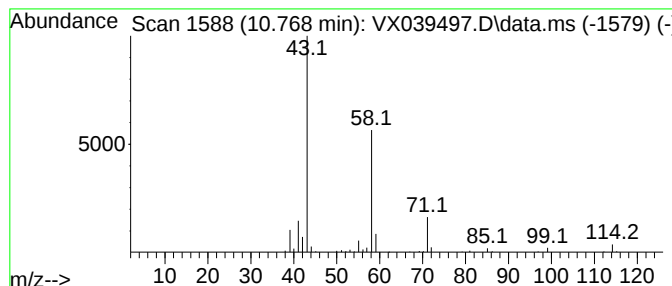
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 2-Heptanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.768	6.59 ug/L	76381	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone			114	C7H14O	000110-43-0	91
2	2-Heptanone			114	C7H14O	000110-43-0	91
3	2-Heptanone			114	C7H14O	000110-43-0	91
4	2-Heptanone			114	C7H14O	000110-43-0	78
5	2-Hexanone, 5-methyl-			114	C7H14O	000110-12-3	64



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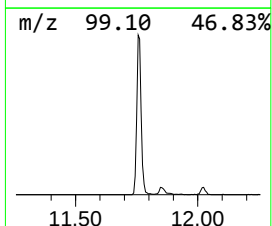
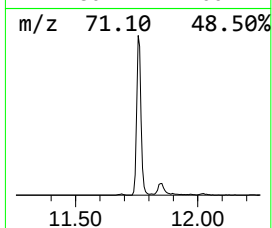
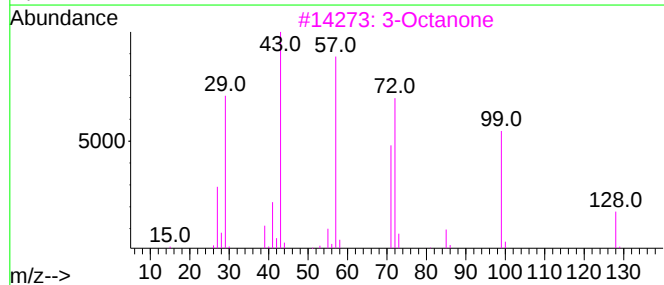
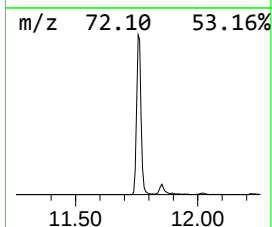
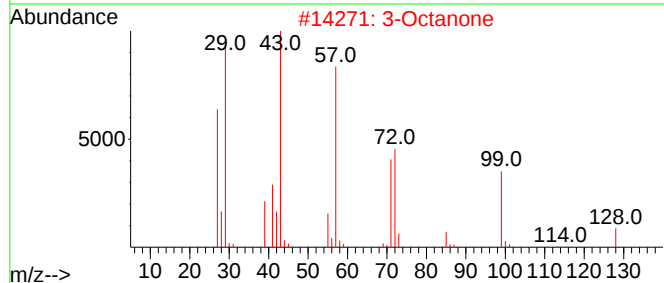
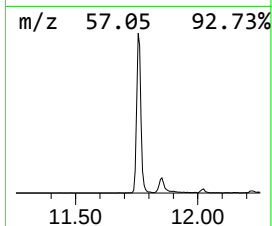
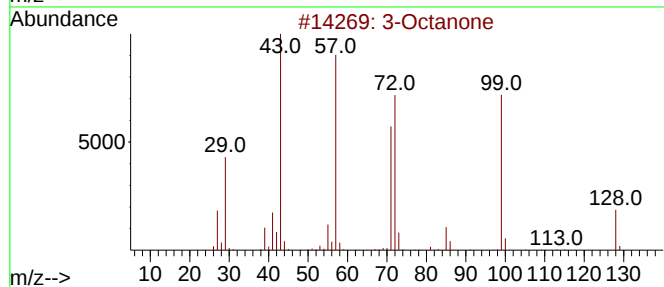
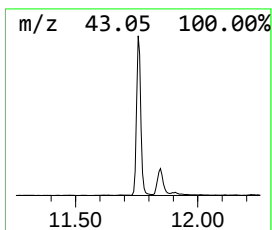
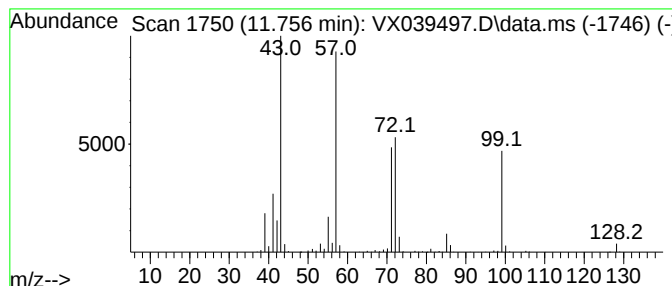
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 3-Octanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.756	35.88 ug/L	423353	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octanone			128	C8H16O	000106-68-3	94
2	3-Octanone			128	C8H16O	000106-68-3	78
3	3-Octanone			128	C8H16O	000106-68-3	47
4	3-Octanone			128	C8H16O	000106-68-3	42
5	6-Undecanone			170	C11H22O	000927-49-1	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122723\
Data File : VX039497.D
Acq On : 27 Dec 2023 15:21
Operator : JC/MD
Sample : 05989-02DL 4X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
F7A61DL

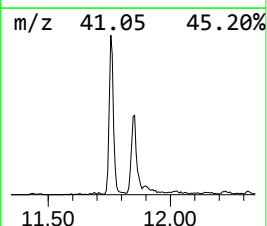
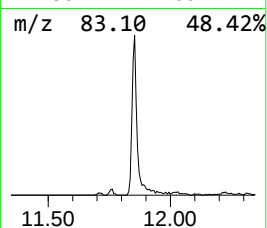
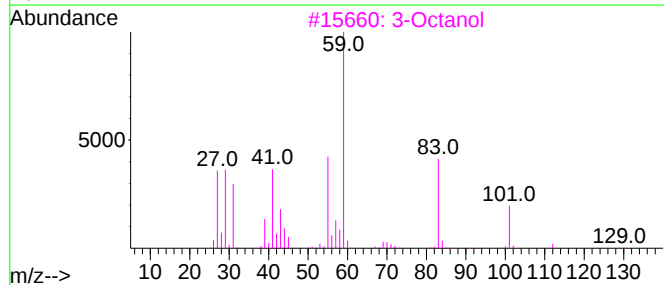
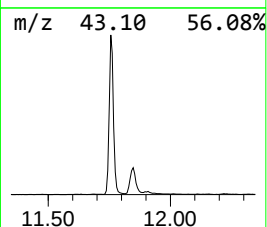
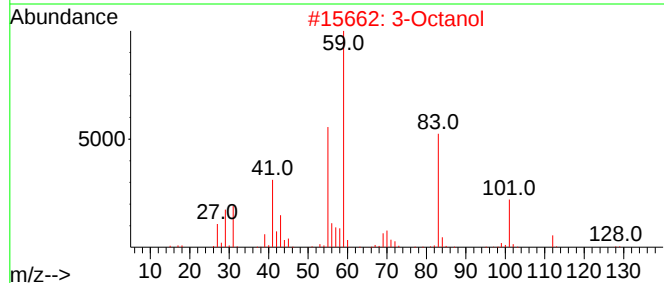
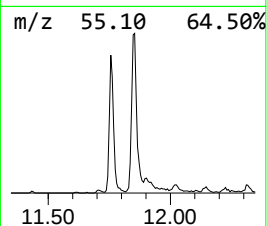
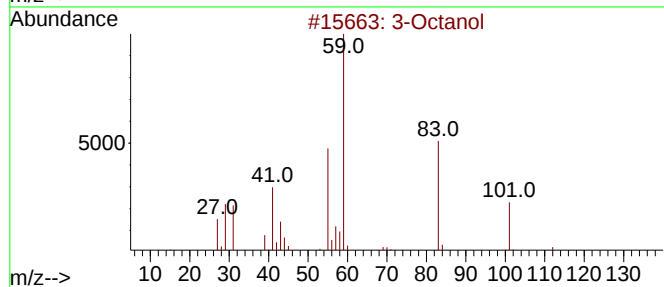
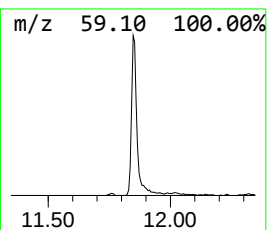
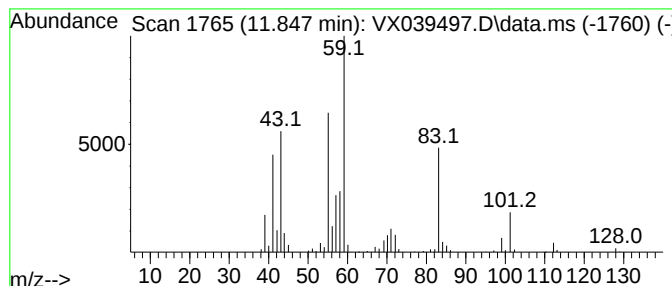
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Quant Title : VOC Analysis

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

Peak Number 5 3-Octanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.847	14.66 ug/L	173010	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octanol			130	C8H18O	000589-98-0	64
2	3-Octanol			130	C8H18O	000589-98-0	64
3	3-Octanol			130	C8H18O	000589-98-0	64
4	3-Octanol			130	C8H18O	000589-98-0	64
5	3-Heptanol, 6-methyl-			130	C8H18O	018720-66-6	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122723\
Data File : VX039497.D
Acq On : 27 Dec 2023 15:21
Operator : JC/MD
Sample : 05989-02DL 4X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
F7A61DL

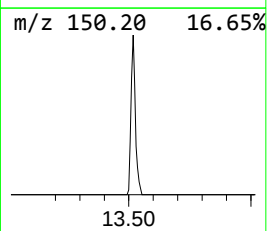
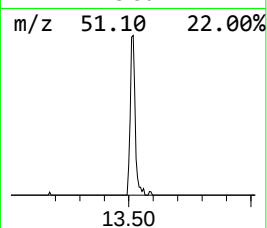
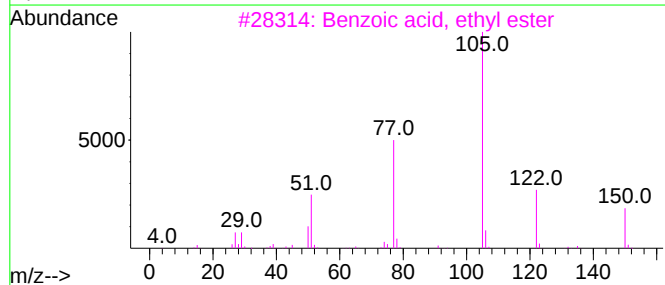
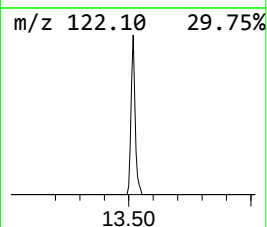
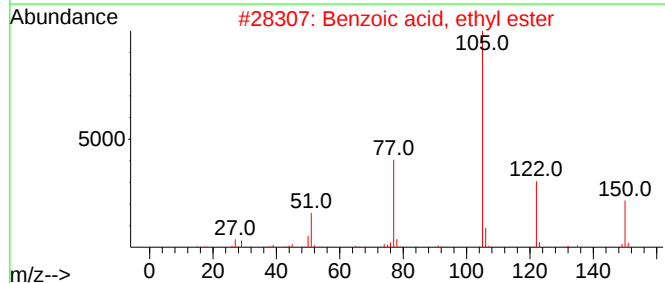
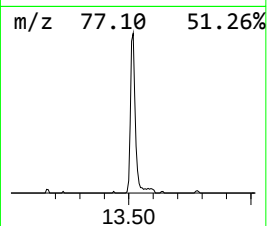
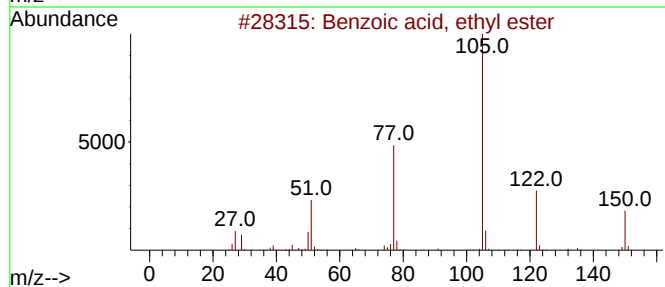
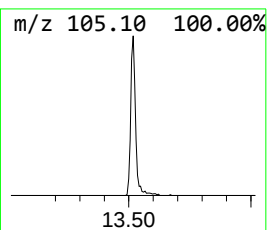
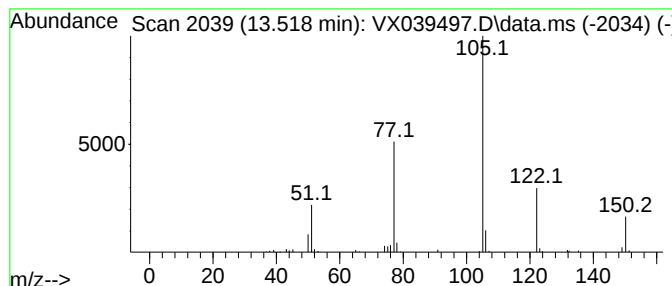
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Quant Title : VOC Analysis

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

Peak Number 6 Benzoic acid, ethyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.518	3.60 ug/L	42448	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, ethyl ester	150	C9H10O2	000093-89-0	91
2			Benzoic acid, ethyl ester	150	C9H10O2	000093-89-0	91
3			Benzoic acid, ethyl ester	150	C9H10O2	000093-89-0	90
4			Benzoic acid, ethyl ester	150	C9H10O2	000093-89-0	70
5			1-Propanone, 3-hydroxy-1-phenyl-	150	C9H10O2	005650-41-9	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122723\
Data File : VX039497.D
Acq On : 27 Dec 2023 15:21
Operator : JC/MD
Sample : 05989-02DL 4X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
F7A61DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120523WMA.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
2-Pentanone	7.464	3.6	ug/L	34233	1	6.763	477409	50.0
2-Heptanone	10.768	6.6	ug/L	76381	2	10.055	579326	50.0
3-Octanone	11.756	35.9	ug/L	423353	3	12.024	589923	50.0
3-Octanol	11.847	14.7	ug/L	173010	3	12.024	589923	50.0
Benzoic acid, e...	13.518	3.6	ug/L	42448	3	12.024	589923	50.0