

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122723\
 Data File : VX039490.D
 Acq On : 27 Dec 2023 12:43
 Operator : JC/MD
 Sample : 05989-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 F7A62

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\SFAMXLM120523WMA.M
 Title : VOC Analysis

Signal : TIC: VX039490.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	32	rBV	6947	15472	0.72%	0.116%
2	1.368	43	46	54	rVB	78217	81491	3.81%	0.612%
3	1.453	57	60	65	rVB	19259	21198	0.99%	0.159%
4	1.666	91	95	104	rVB	54017	80105	3.75%	0.601%
5	2.057	154	159	168	rVB	26084	43466	2.03%	0.326%
6	2.307	193	200	206	rBV	149264	232941	10.89%	1.748%
7	2.374	206	211	216	rVV	133525	221343	10.35%	1.661%
8	2.422	216	219	229	rVB	67687	104250	4.88%	0.782%
9	2.532	230	237	248	rVV	56665	106324	4.97%	0.798%
10	2.703	260	265	273	rVB	6815	13052	0.61%	0.098%
11	2.788	277	279	284	rVB3	791	699	0.03%	0.005%
12	2.867	290	292	295	rVB3	449	442	0.02%	0.003%
13	2.953	299	306	313	rVB6	1653	4328	0.20%	0.032%
14	3.014	315	316	322	rVB	492	487	0.02%	0.004%
15	3.063	322	324	326	rBV2	373	342	0.02%	0.003%
16	3.331	364	368	375	rVV2	1184	2135	0.10%	0.016%
17	3.843	448	452	453	rBV	4156	4379	0.20%	0.033%
18	4.007	476	479	486	rBV3	769	1390	0.07%	0.010%
19	4.245	512	518	527	rVB4	1543	4255	0.20%	0.032%
20	4.355	529	536	537	rBV4	1682	2549	0.12%	0.019%
21	4.453	543	552	560	rBV	102011	336693	15.74%	2.527%
22	4.550	561	568	590	rVB	423059	1193588	55.82%	8.958%
23	4.989	628	640	646	rBV	161721	495904	23.19%	3.722%
24	5.465	716	718	721	rVB3	481	359	0.02%	0.003%
25	5.733	758	762	766	rBV3	250	416	0.02%	0.003%
26	5.971	789	801	818	rBV2	248078	758409	35.47%	5.692%
27	6.123	819	826	832	rBV3	5141	12877	0.60%	0.097%
28	6.574	898	900	903	rBV2	203	310	0.01%	0.002%
29	6.757	921	930	947	rBV	215201	521244	24.38%	3.912%
30	6.952	959	962	964	rBV2	399	364	0.02%	0.003%
31	7.019	968	973	978	rVV4	804	1751	0.08%	0.013%
32	7.141	987	993	997	rBV7	1553	3287	0.15%	0.025%
33	7.208	997	1004	1012	rVV	55716	123893	5.79%	0.930%
34	7.306	1013	1020	1034	rVV	167058	376766	17.62%	2.828%
35	7.452	1038	1044	1061	rVV	88596	184441	8.63%	1.384%
36	7.592	1061	1067	1070	rVV3	4060	8725	0.41%	0.065%

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Integrator: RTE

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

37	7.641	1070	1075	1089	rVB	19530	40264	1.88%	0.302%
38	7.903	1111	1118	1134	rBV2	26234	66555	3.11%	0.499%
39	8.324	1181	1187	1195	rBV	110845	177169	8.29%	1.330%
40	8.574	1222	1228	1234	rBV	21763	36215	1.69%	0.272%
41	8.647	1234	1240	1248	rBV	366086	575516	26.91%	4.319%
42	8.952	1284	1290	1300	rBV	78029	119481	5.59%	0.897%
43	9.165	1323	1325	1330	rVB5	821	1198	0.06%	0.009%
44	9.238	1332	1337	1340	rBV2	6326	10233	0.48%	0.077%
45	9.342	1347	1354	1356	rBV3	15611	21467	1.00%	0.161%
46	9.385	1356	1361	1366	rBV	426818	591864	27.68%	4.442%
47	9.519	1380	1383	1391	rBV	11434	17146	0.80%	0.129%
48	9.756	1421	1422	1423	rBV	597	375	0.02%	0.003%
49	10.055	1463	1471	1483	rBV	451200	643396	30.09%	4.829%
50	10.159	1485	1488	1493	rVB3	3071	4209	0.20%	0.032%
51	10.269	1504	1506	1516	rVB7	2414	4616	0.22%	0.035%
52	10.384	1523	1525	1527	rVV	1193	1159	0.05%	0.009%
53	10.415	1527	1530	1534	rVB5	1437	2271	0.11%	0.017%
54	10.506	1539	1545	1550	rBV4	1289	2536	0.12%	0.019%
55	10.579	1553	1557	1565	rBV	27253	44629	2.09%	0.335%
56	10.768	1583	1588	1598	rBV	294476	376458	17.60%	2.825%
57	10.878	1601	1606	1616	rVV	102428	147100	6.88%	1.104%
58	11.085	1636	1640	1644	rVB5	3150	4497	0.21%	0.034%
59	11.189	1652	1657	1667	rVB	340669	431526	20.18%	3.239%
60	11.433	1693	1697	1703	rBV3	4634	6251	0.29%	0.047%
61	11.482	1703	1705	1710	rVB4	1198	1508	0.07%	0.011%
62	11.591	1719	1723	1727	rBV2	3593	5621	0.26%	0.042%
63	11.683	1735	1738	1740	rBV2	4319	5635	0.26%	0.042%
64	11.756	1745	1750	1759	rVV	1858891	2138413	100.00%	16.048%
65	11.848	1759	1765	1771	rVV2	876798	1118683	52.31%	8.395%
66	11.896	1771	1773	1788	rVV	66463	127811	5.98%	0.959%
67	12.018	1788	1793	1802	rVB	492424	644256	30.13%	4.835%
68	12.140	1810	1813	1821	rVB4	12542	19654	0.92%	0.147%
69	12.219	1822	1826	1834	rBV	18691	31336	1.47%	0.235%
70	12.317	1837	1842	1848	rVV	434121	548879	25.67%	4.119%
71	12.561	1879	1882	1884	rBV2	4063	4424	0.21%	0.033%
72	12.689	1900	1903	1911	rVB3	7448	10071	0.47%	0.076%
73	12.768	1911	1916	1919	rBV	30496	40678	1.90%	0.305%
74	13.164	1976	1981	1990	rBV	14923	26384	1.23%	0.198%
75	13.402	2018	2020	2022	rBV2	1218	1334	0.06%	0.010%
76	13.445	2024	2027	2034	rVV3	6344	8595	0.40%	0.065%

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 Title : VOC Analysis

77	13.512	2034	2038	2046	rVV	204055	255034	11.93%	1.914%
78	13.774	2078	2081	2086	rVB	4392	5082	0.24%	0.038%
79	13.890	2097	2100	2106	rBV4	1209	2002	0.09%	0.015%
80	13.963	2110	2112	2114	rVB2	611	343	0.02%	0.003%
81	14.061	2126	2128	2132	rVB4	1192	1005	0.05%	0.008%
82	14.115	2134	2137	2142	rVV2	1462	1977	0.09%	0.015%
83	14.195	2146	2150	2153	rBV3	759	1016	0.05%	0.008%
84	14.262	2158	2161	2162	rBV3	437	340	0.02%	0.003%
85	14.298	2162	2167	2171	rBV2	5980	7993	0.37%	0.060%
86	14.371	2176	2179	2184	rVV5	3489	4790	0.22%	0.036%
87	14.420	2185	2187	2195	rVB3	1266	1951	0.09%	0.015%
88	14.512	2198	2202	2208	rVB3	4764	6569	0.31%	0.049%
89	14.640	2220	2223	2226	rVB3	2309	3156	0.15%	0.024%
90	14.780	2242	2246	2250	rVB3	1465	2084	0.10%	0.016%
91	14.908	2263	2267	2270	rVB4	1624	2175	0.10%	0.016%
92	15.024	2284	2286	2287	rBV2	321	344	0.02%	0.003%
93	15.054	2287	2291	2294	rVV2	2192	2816	0.13%	0.021%
94	15.158	2305	2308	2310	rBV3	509	720	0.03%	0.005%
95	15.182	2310	2312	2315	rVV3	366	415	0.02%	0.003%
96	15.566	2371	2375	2380	rVB4	1725	2910	0.14%	0.022%
97	16.164	2468	2473	2477	rVB5	1025	1728	0.08%	0.013%
98	16.213	2480	2481	2484	rBV3	490	525	0.02%	0.004%
99	16.463	2519	2522	2525	rVB3	355	410	0.02%	0.003%
100	16.755	2568	2570	2573	rVB2	330	324	0.02%	0.002%

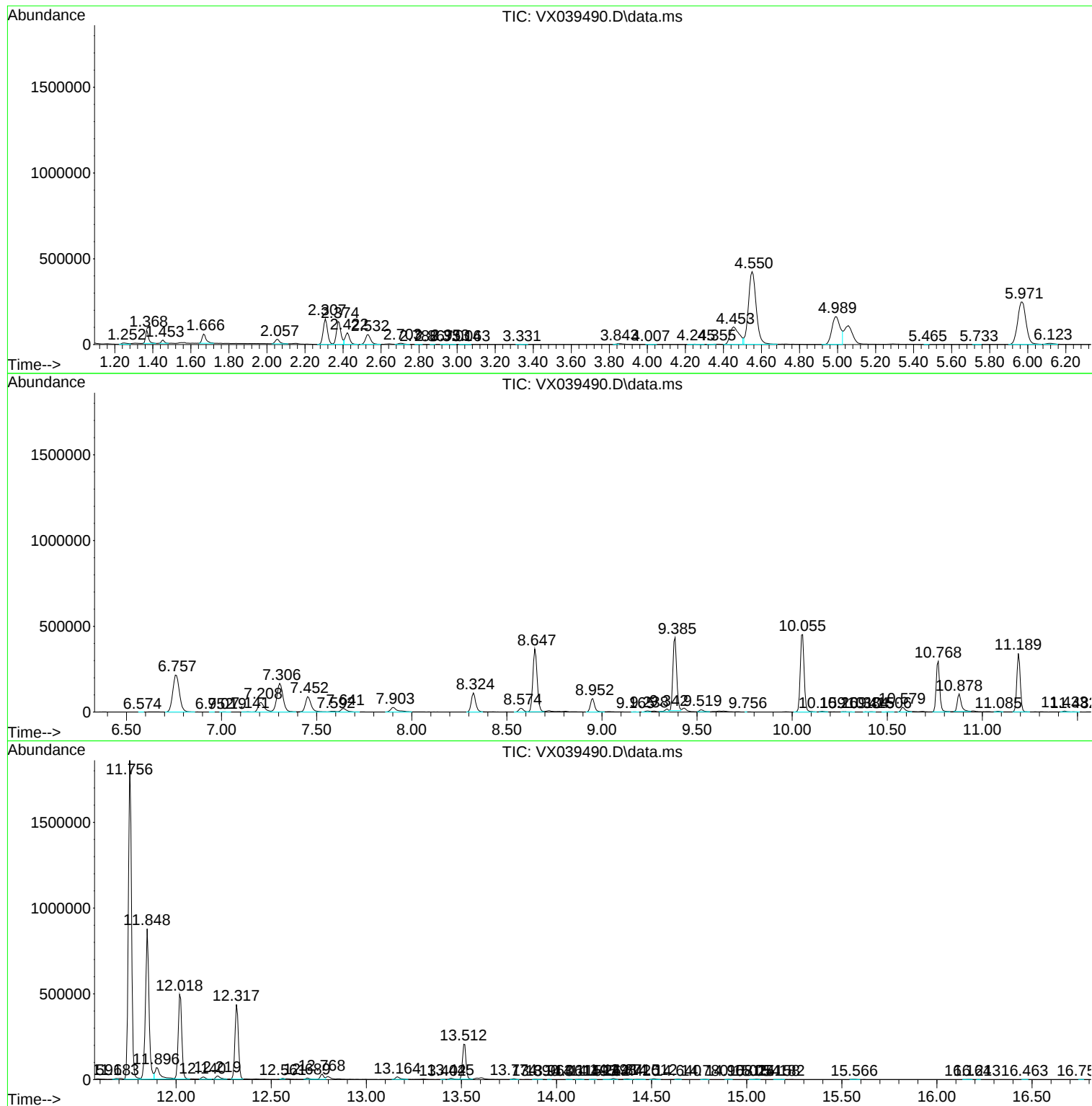
Sum of corrected areas: 13324797

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Instrument :
MSVOA_X
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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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122723\
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Instrument :
MSVOA_X
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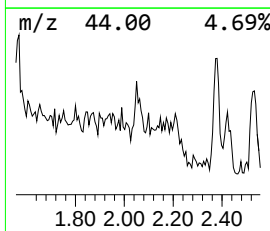
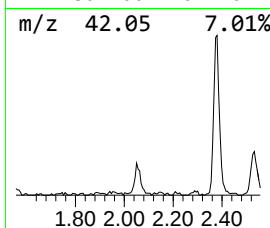
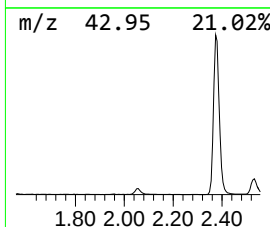
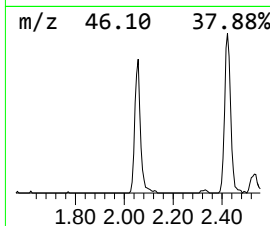
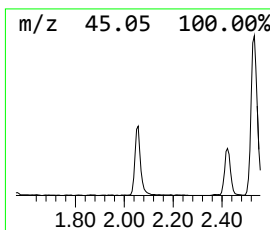
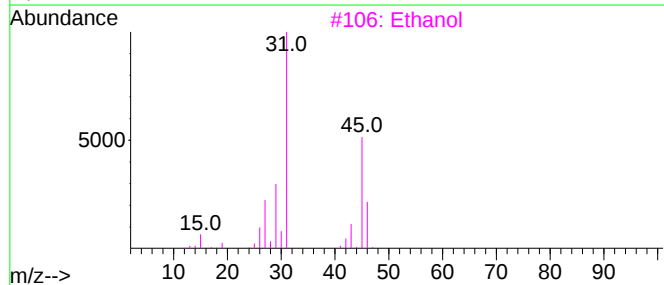
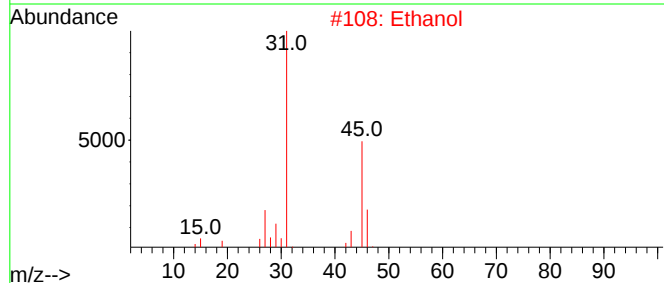
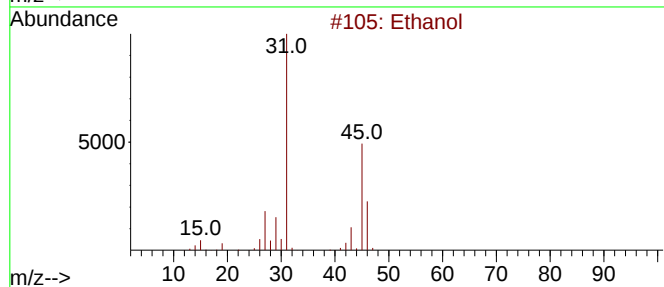
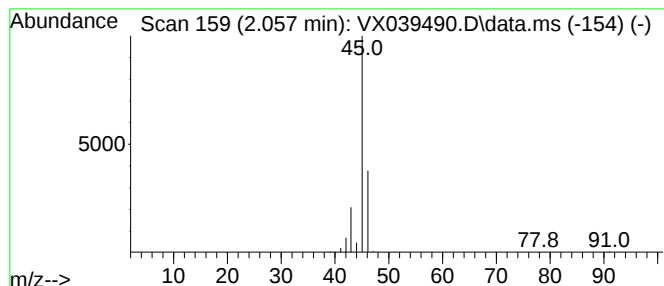
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.057	4.17 ug/L	43466	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	43
2	Ethanol			46	C2H6O	000064-17-5	9
3	Ethanol			46	C2H6O	000064-17-5	9
4	Dimethyl ether			46	C2H6O	000115-10-6	9
5	Ethanol			46	C2H6O	000064-17-5	9



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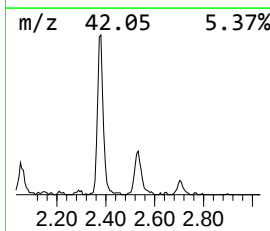
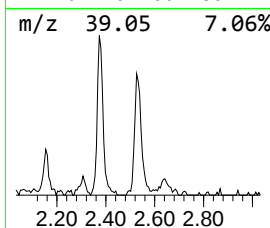
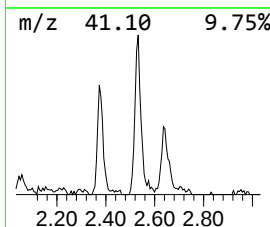
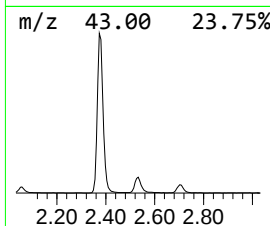
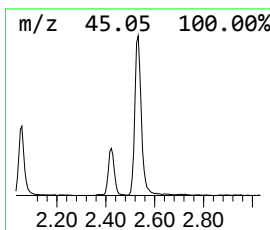
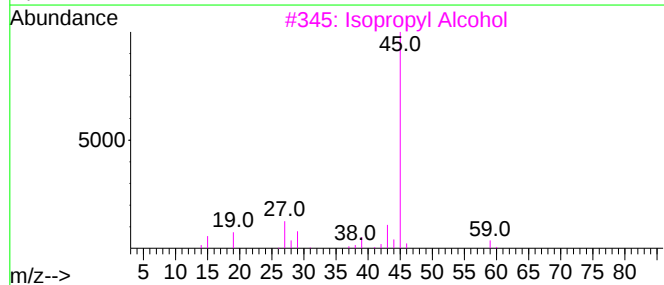
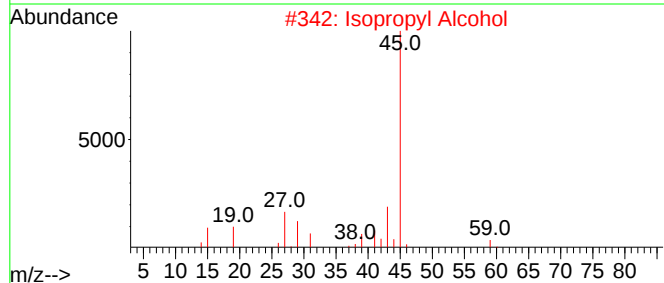
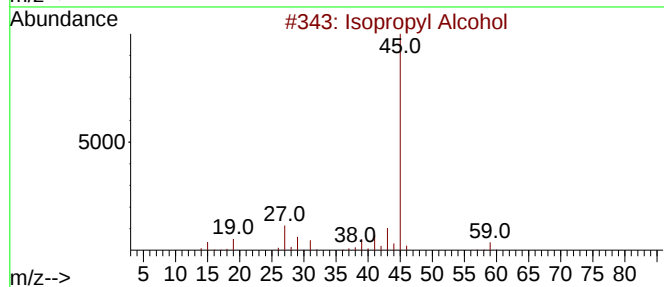
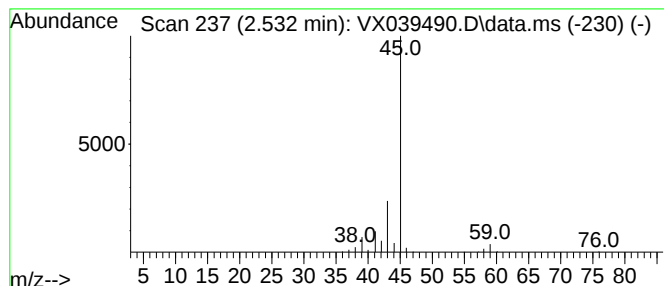
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Isopropyl Alcohol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.532	10.20 ug/L	106324	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	86
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
5			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	40



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ALS Vial : 7 Sample Multiplier: 1

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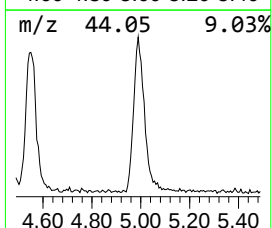
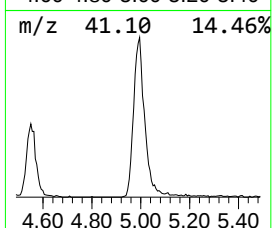
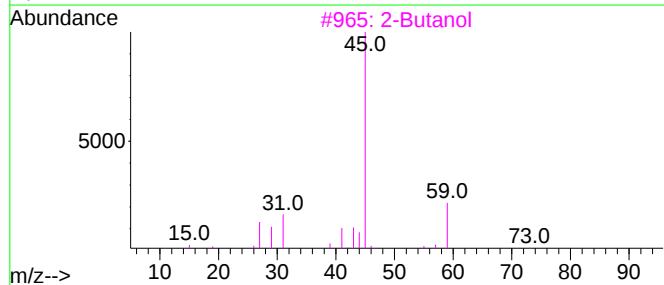
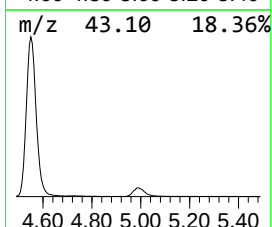
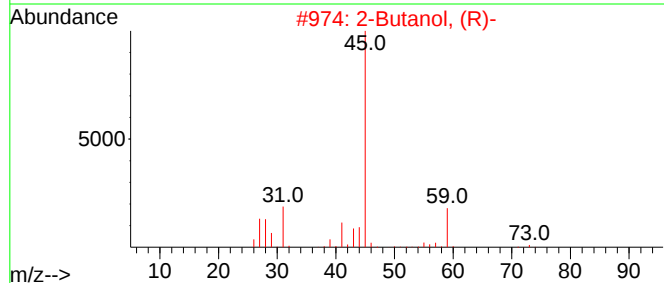
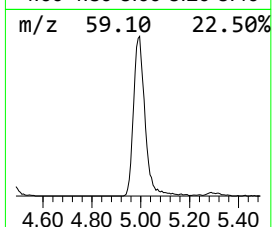
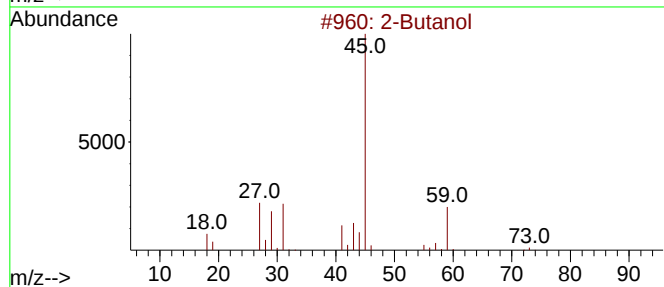
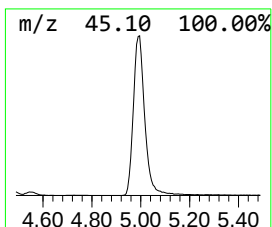
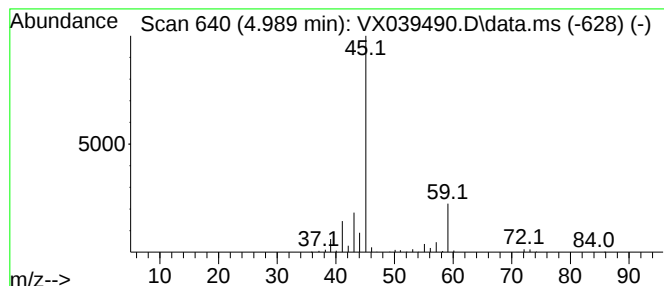
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 2-Butanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.989	47.57 ug/L	495904	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol			74	C4H10O	000078-92-2	83
2	2-Butanol, (R)-			74	C4H10O	014898-79-4	83
3	2-Butanol			74	C4H10O	000078-92-2	83
4	2-Butanol			74	C4H10O	000078-92-2	83
5	2-Butanol, (R)-			74	C4H10O	014898-79-4	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122723\
Data File : VX039490.D
Acq On : 27 Dec 2023 12:43
Operator : JC/MD
Sample : 05989-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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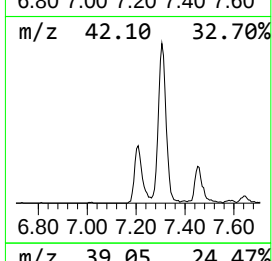
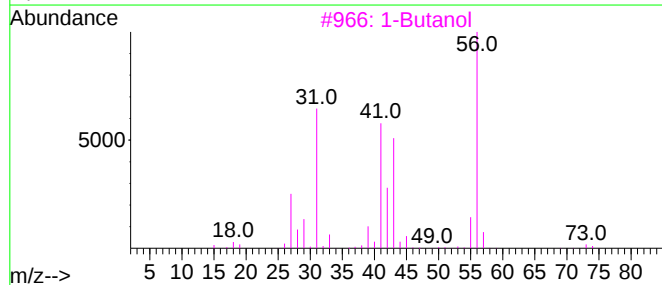
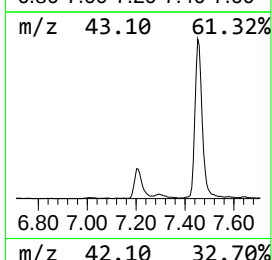
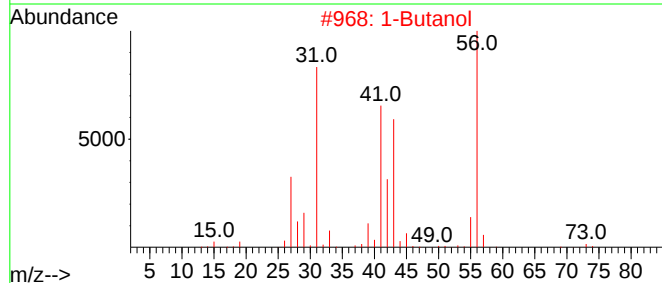
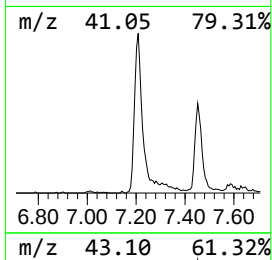
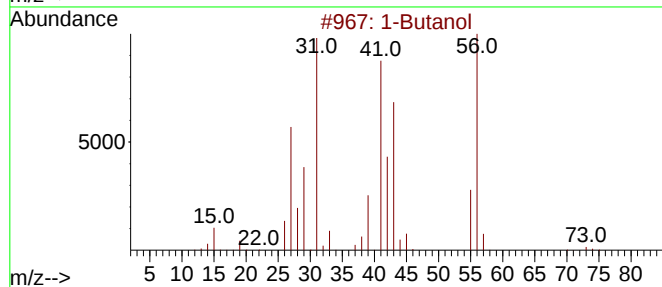
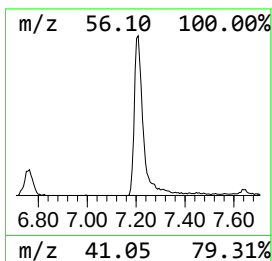
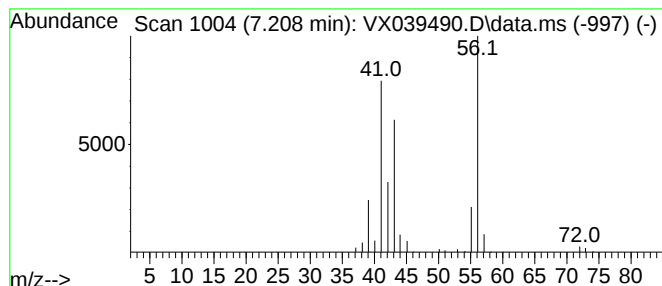
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Quant Title : VOC Analysis

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

Peak Number 4 1-Butanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	11.88 ug/L	123893	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol			74	C4H10O	000071-36-3	90
2	1-Butanol			74	C4H10O	000071-36-3	90
3	1-Butanol			74	C4H10O	000071-36-3	83
4	1-Butanol			74	C4H10O	000071-36-3	80
5	1-Butanol			74	C4H10O	000071-36-3	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122723\
Data File : VX039490.D
Acq On : 27 Dec 2023 12:43
Operator : JC/MD
Sample : 05989-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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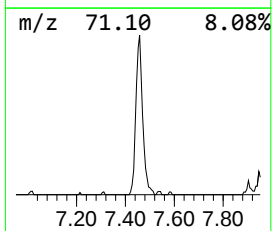
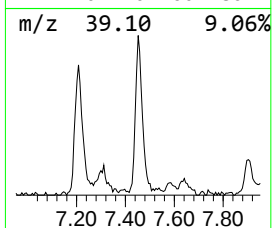
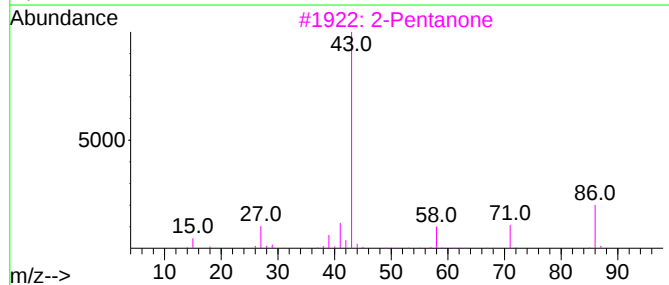
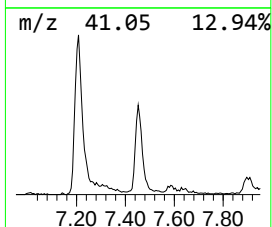
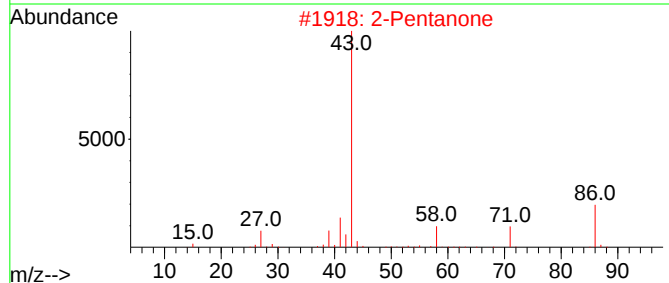
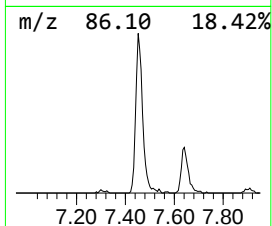
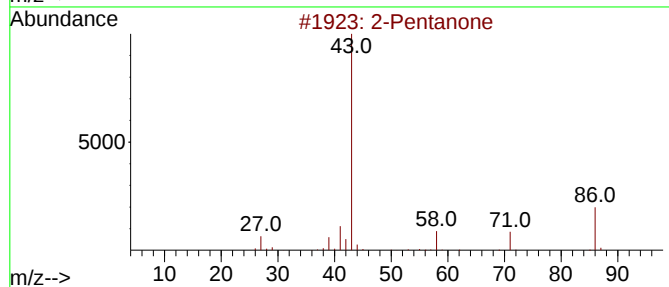
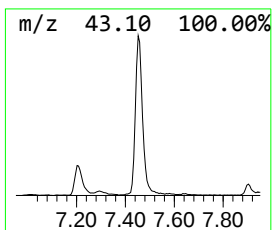
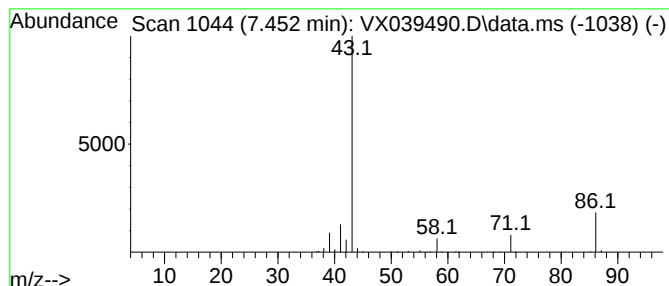
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Quant Title : VOC Analysis

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

Peak Number 5 2-Pentanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.452	17.69 ug/L	184441	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone			86	C5H10O	000107-87-9	72
2	2-Pentanone			86	C5H10O	000107-87-9	58
3	2-Pentanone			86	C5H10O	000107-87-9	58
4	2-Butanone, 3-methyl-			86	C5H10O	000563-80-4	53
5	2-Butanone, 3-methyl-			86	C5H10O	000563-80-4	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122723\
Data File : VX039490.D
Acq On : 27 Dec 2023 12:43
Operator : JC/MD
Sample : 05989-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
F7A62

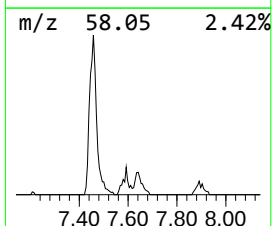
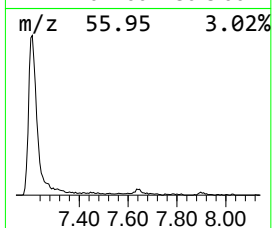
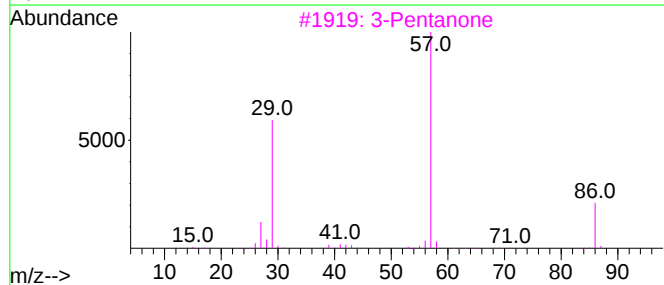
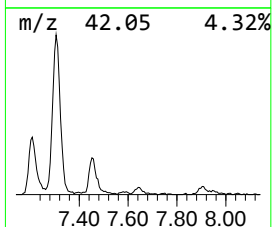
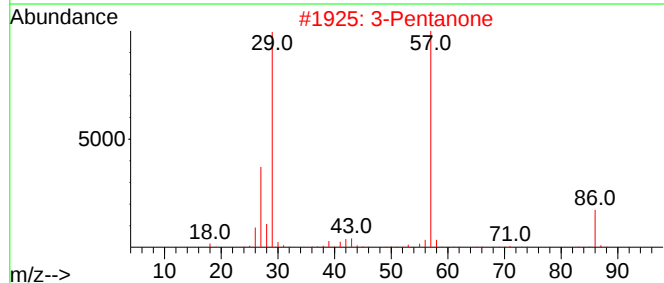
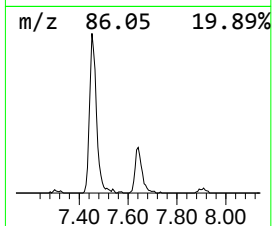
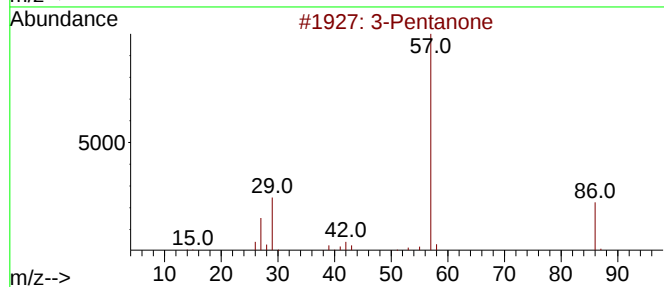
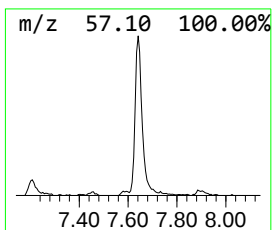
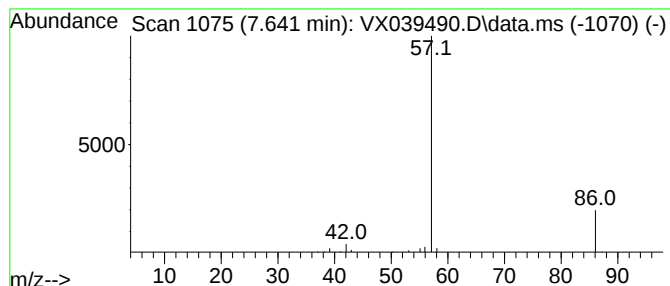
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Quant Title : VOC Analysis

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

Peak Number 6 3-Pentanone Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.641	3.86 ug/L	40264	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone			86	C5H10O	000096-22-0	78
2	3-Pentanone			86	C5H10O	000096-22-0	78
3	3-Pentanone			86	C5H10O	000096-22-0	9
4	3-Pentanone			86	C5H10O	000096-22-0	9
5	Ethyl-1-propenyl ether			86	C5H10O	000928-55-2	7



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122723\
Data File : VX039490.D
Acq On : 27 Dec 2023 12:43
Operator : JC/MD
Sample : 05989-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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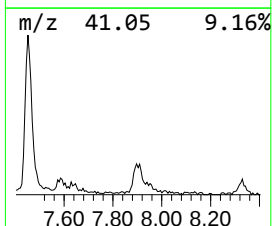
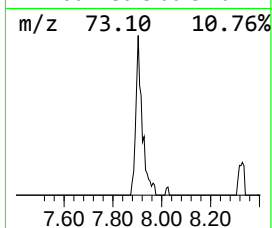
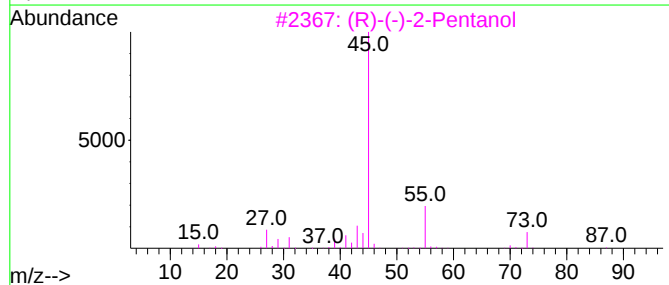
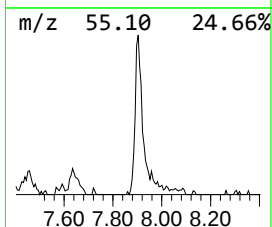
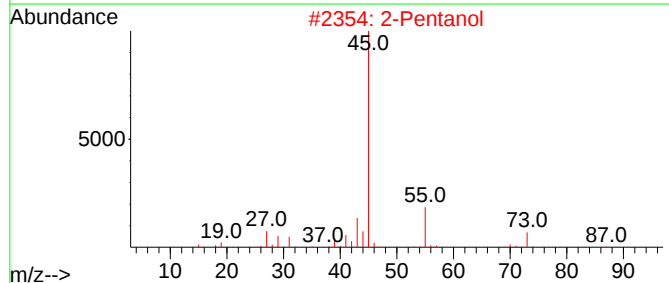
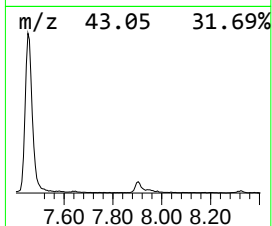
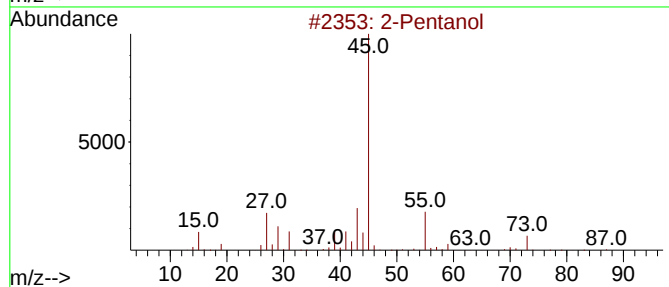
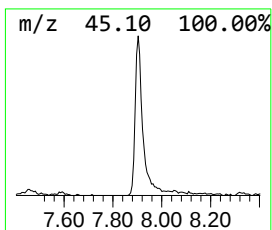
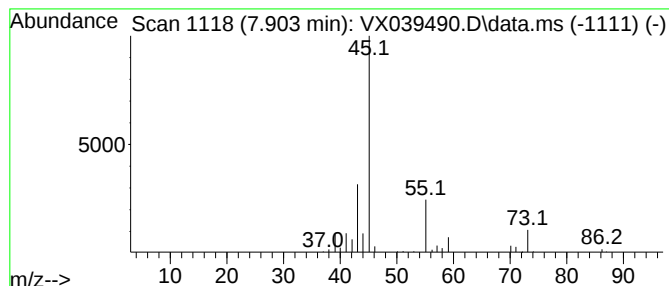
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Quant Title : VOC Analysis

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

Peak Number 7 2-Pentanol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.903	6.38 ug/L	66555	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanol	88	C5H12O	006032-29-7	74
2			2-Pentanol	88	C5H12O	006032-29-7	72
3			(R)-(-)-2-Pentanol	88	C5H12O	031087-44-2	72
4			(S)-(+)-2-Pentanol	88	C5H12O	026184-62-3	72
5			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122723\
Data File : VX039490.D
Acq On : 27 Dec 2023 12:43
Operator : JC/MD
Sample : 05989-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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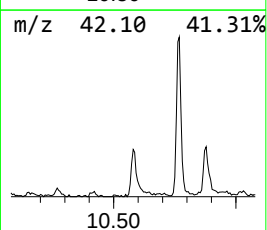
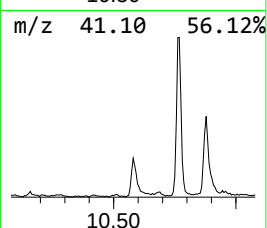
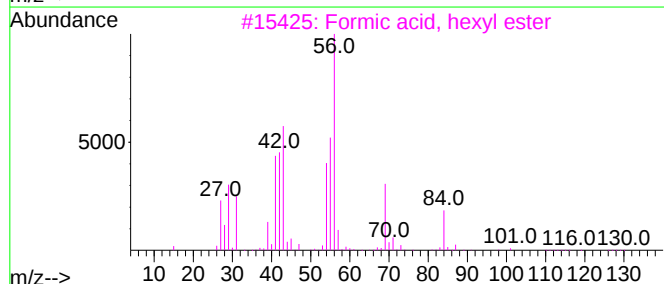
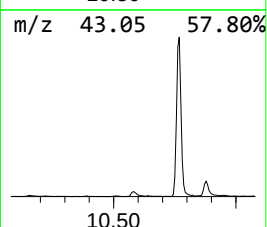
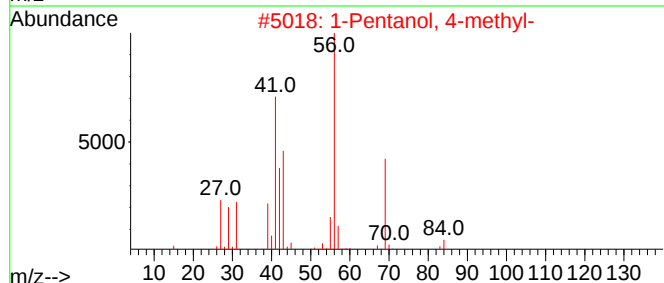
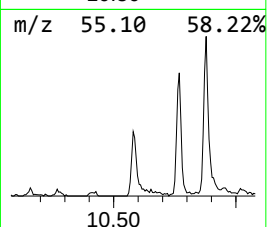
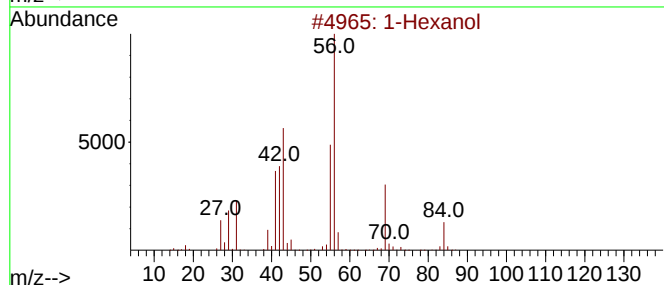
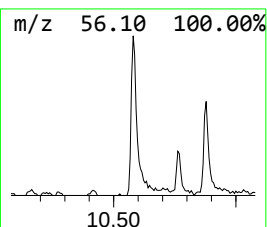
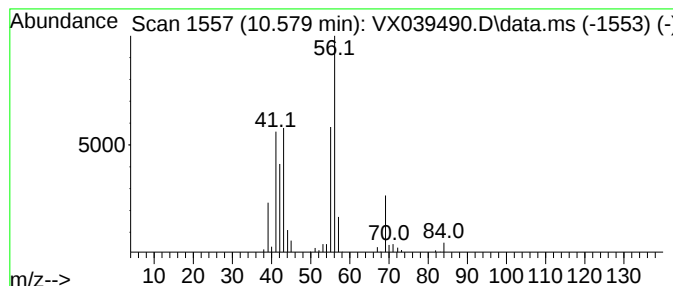
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Quant Title : VOC Analysis

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

Peak Number 9 1-Hexanol Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.579	3.47 ug/L	44629	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol			102	C6H14O	000111-27-3	64
2	1-Pentanol, 4-methyl-			102	C6H14O	000626-89-1	64
3	Formic acid, hexyl ester			130	C7H14O2	000629-33-4	64
4	1-Hexanol			102	C6H14O	000111-27-3	64
5	1-Hexanol			102	C6H14O	000111-27-3	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122723\
Data File : VX039490.D
Acq On : 27 Dec 2023 12:43
Operator : JC/MD
Sample : 05989-03
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ALS Vial : 7 Sample Multiplier: 1

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ClientSampleId :
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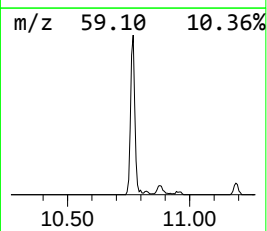
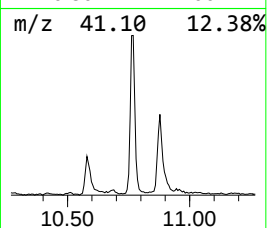
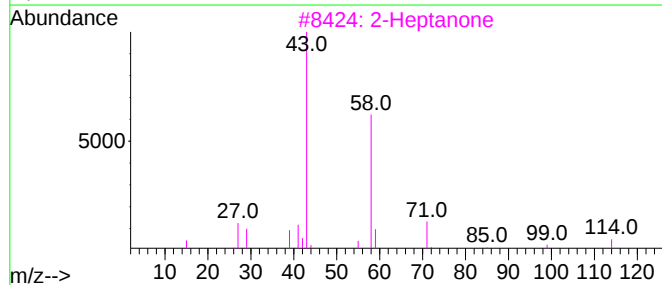
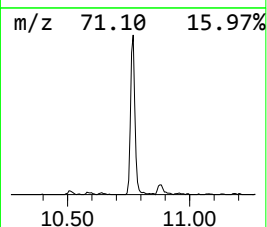
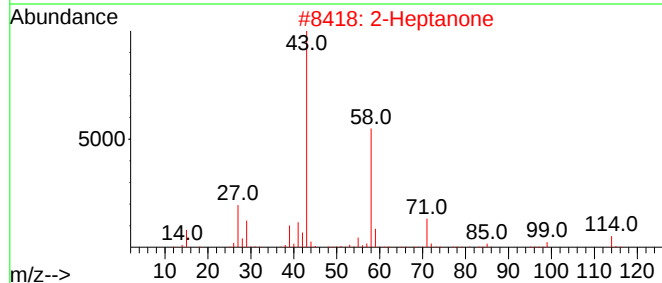
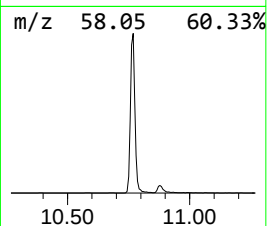
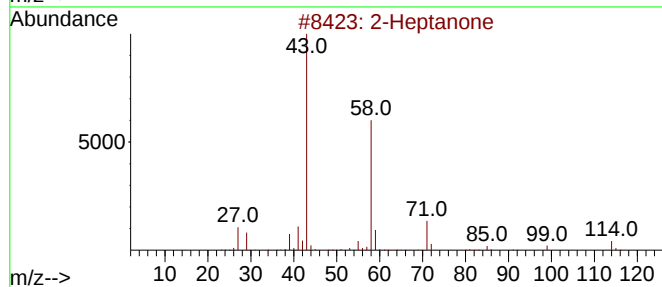
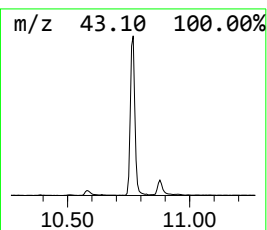
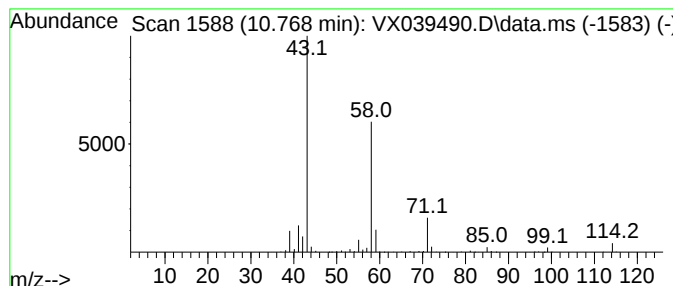
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Quant Title : VOC Analysis

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

Peak Number 10 2-Heptanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.769	29.26 ug/L	376458	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	90
5		2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122723\
Data File : VX039490.D
Acq On : 27 Dec 2023 12:43
Operator : JC/MD
Sample : 05989-03
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ALS Vial : 7 Sample Multiplier: 1

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ClientSampleId :
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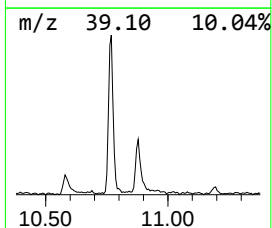
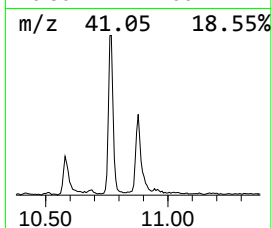
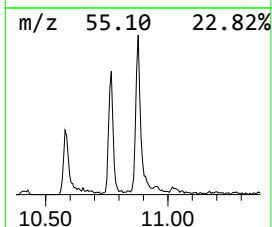
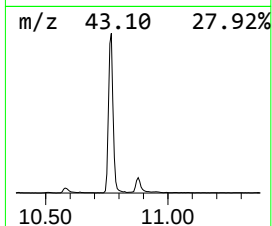
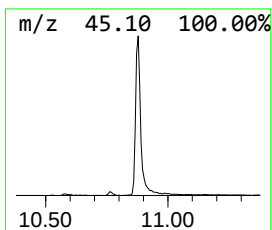
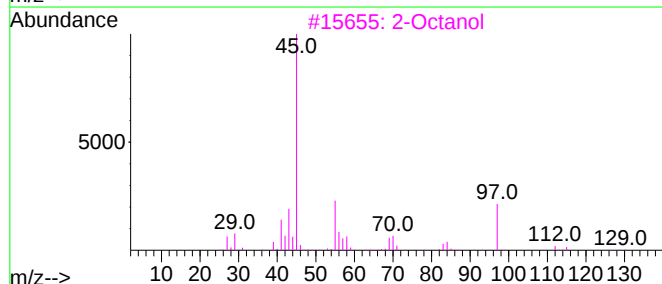
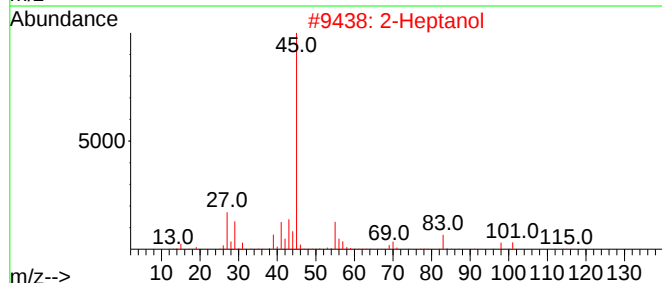
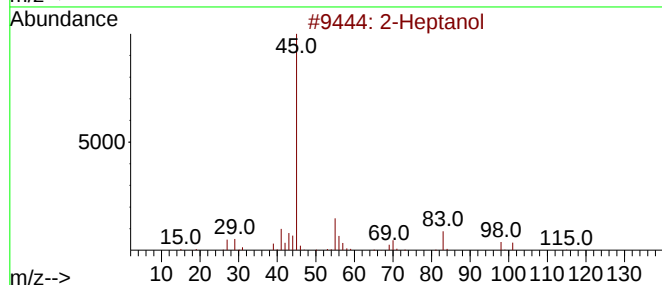
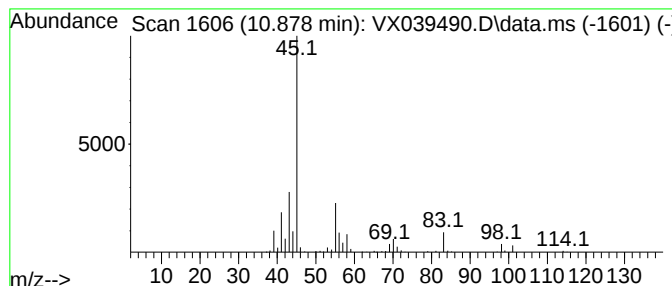
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Quant Title : VOC Analysis

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

Peak Number 11 2-Heptanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.878	11.43 ug/L	147100	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptanol	116	C7H16O	000543-49-7	83
2			2-Heptanol	116	C7H16O	000543-49-7	83
3			2-Octanol	130	C8H18O	000123-96-6	64
4			2-Octanol	130	C8H18O	000123-96-6	64
5			2-Octanol, (S)-	130	C8H18O	006169-06-8	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122723\
Data File : VX039490.D
Acq On : 27 Dec 2023 12:43
Operator : JC/MD
Sample : 05989-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
F7A62

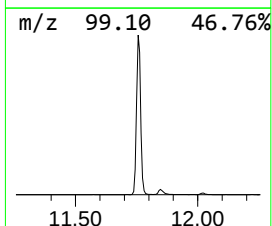
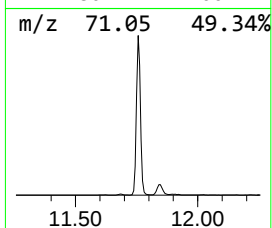
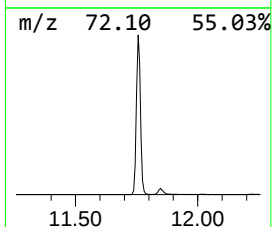
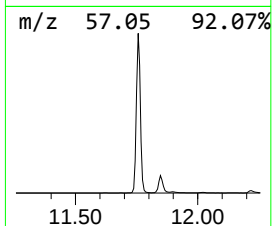
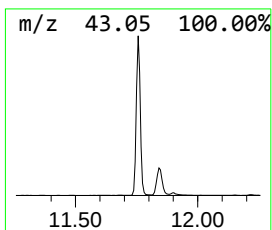
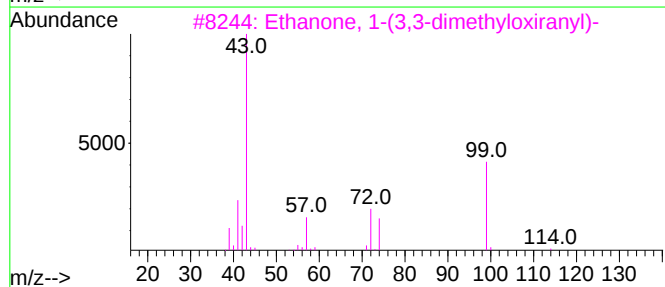
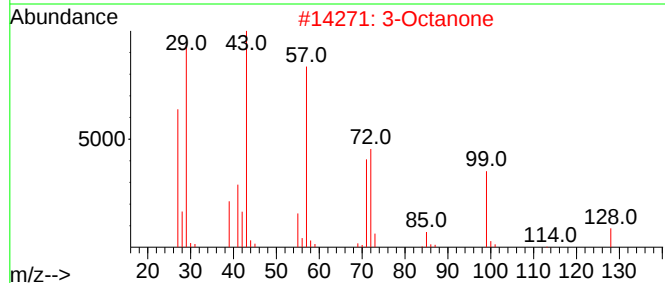
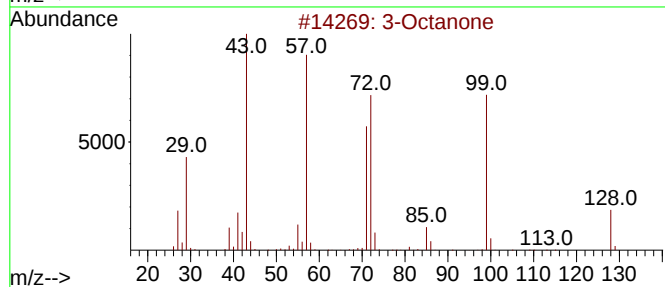
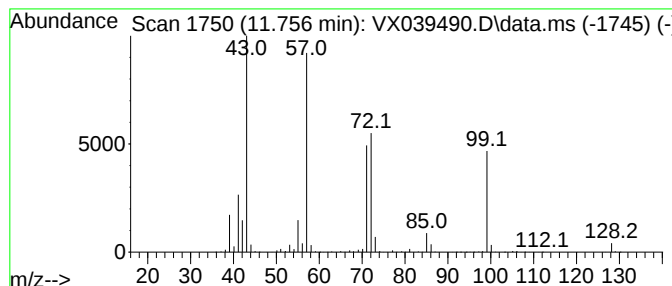
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Quant Title : VOC Analysis

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

Peak Number 12 3-Octanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.756	165.96 ug/L	2138410	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	64
3		Ethanone, 1-(3,3-dimethyloxiranyl)-	114	C6H10O2	004478-63-1	50
4		2-Pentene, 5-(pentyloxy)-, (E)-	156	C10H20O	056052-85-8	47
5		3-Octanone	128	C8H16O	000106-68-3	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122723\
Data File : VX039490.D
Acq On : 27 Dec 2023 12:43
Operator : JC/MD
Sample : 05989-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

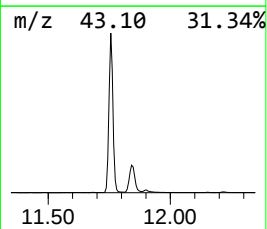
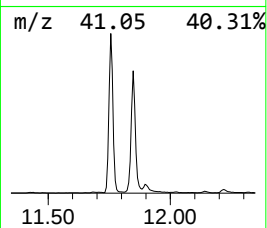
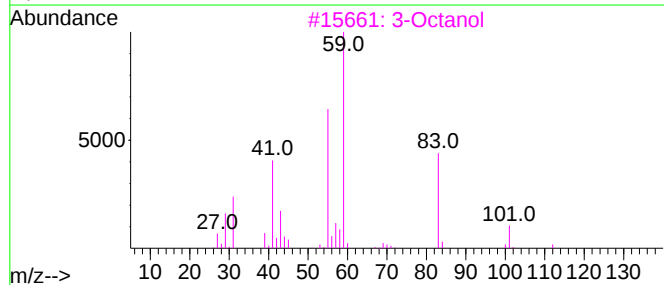
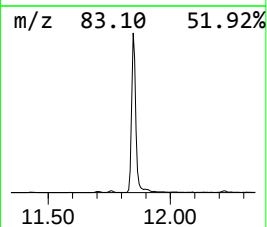
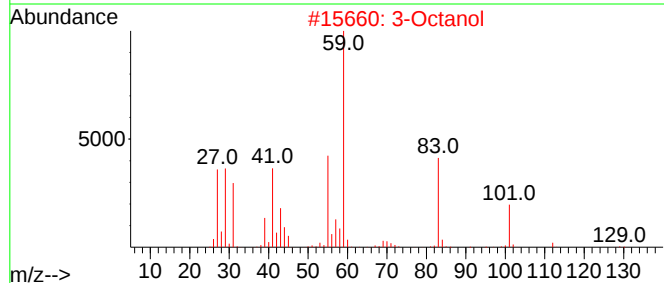
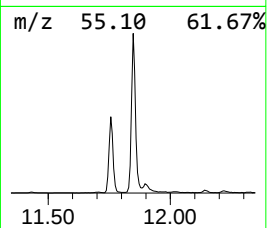
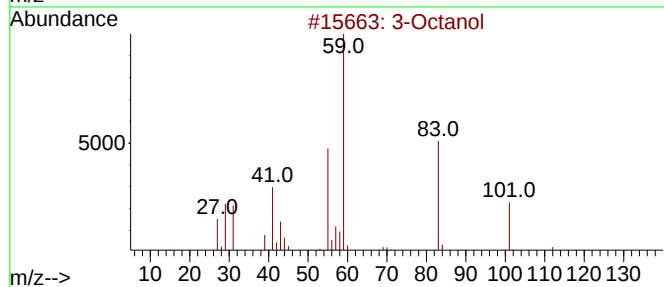
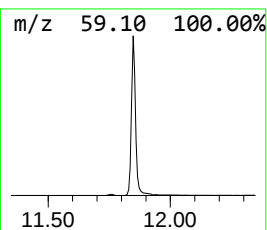
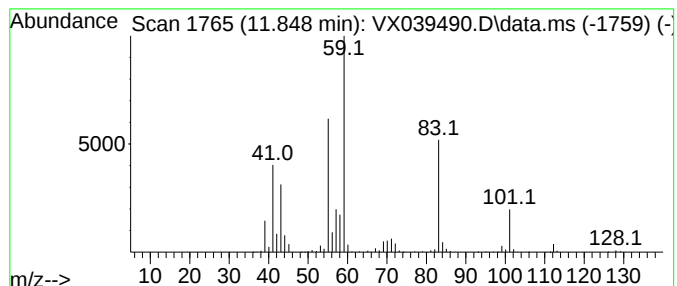
Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 13 3-Octanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD			R.T.
11.848	86.82 ug/L	1118680	1,4-Dichlorobenzene-d4			12.024
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	3-Octanol		130	C8H18O	000589-98-0	90
2	3-Octanol		130	C8H18O	000589-98-0	83
3	3-Octanol		130	C8H18O	000589-98-0	78
4	3-Heptanol, 6-methyl-		130	C8H18O	018720-66-6	72
5	3-Octanol		130	C8H18O	000589-98-0	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122723\
Data File : VX039490.D
Acq On : 27 Dec 2023 12:43
Operator : JC/MD
Sample : 05989-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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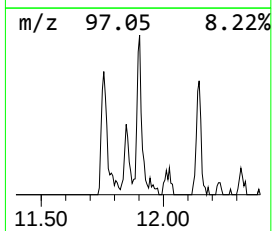
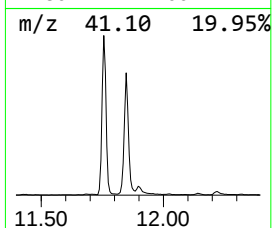
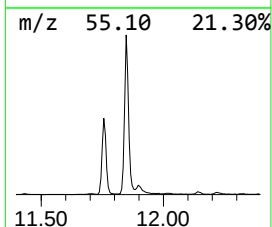
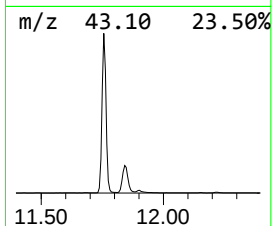
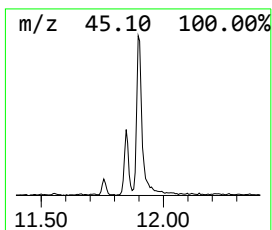
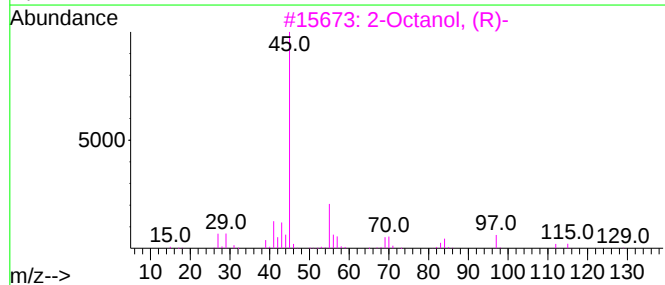
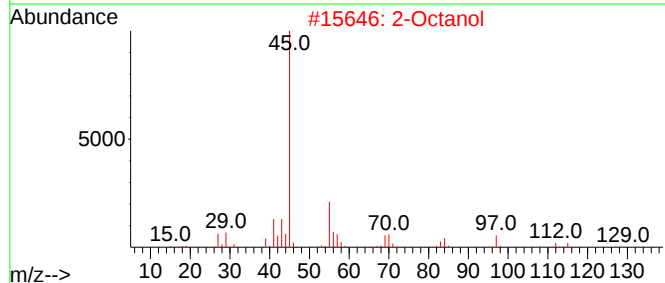
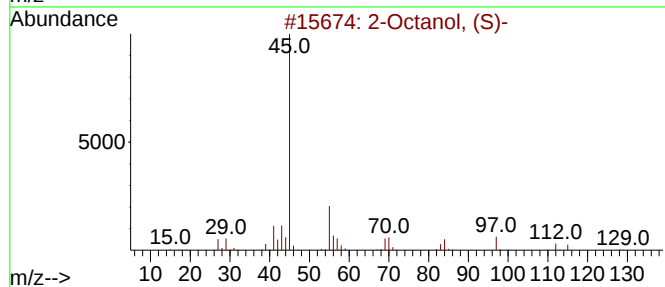
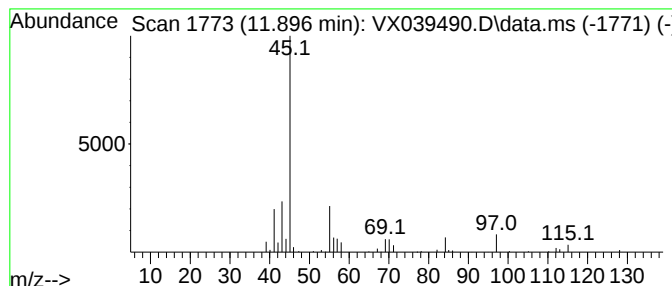
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Quant Title : VOC Analysis

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

Peak Number 14 2-Octanol, (S)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.896	9.92 ug/L	127811	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octanol, (S)-			130	C8H18O	006169-06-8	86
2	2-Octanol			130	C8H18O	000123-96-6	83
3	2-Octanol, (R)-			130	C8H18O	005978-70-1	83
4	2-Octanol, (S)-			130	C8H18O	006169-06-8	78
5	2-Octanol, (R)-			130	C8H18O	005978-70-1	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122723\
Data File : VX039490.D
Acq On : 27 Dec 2023 12:43
Operator : JC/MD
Sample : 05989-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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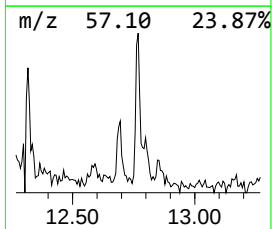
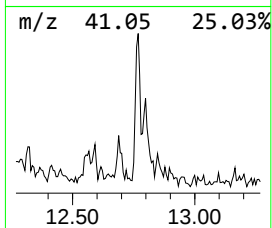
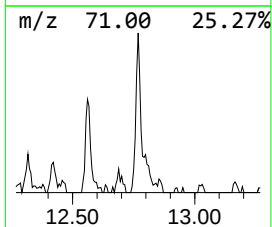
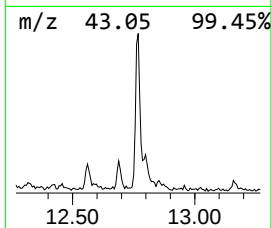
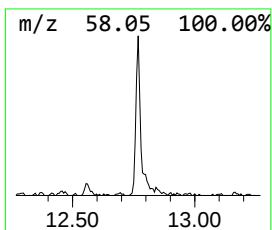
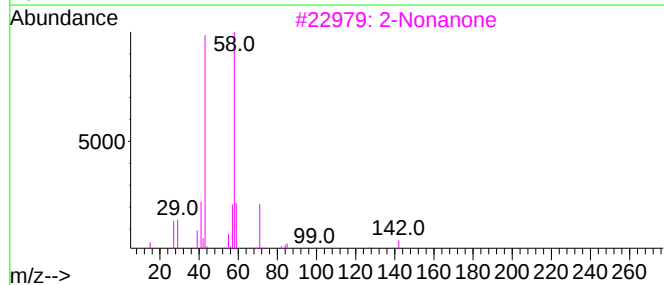
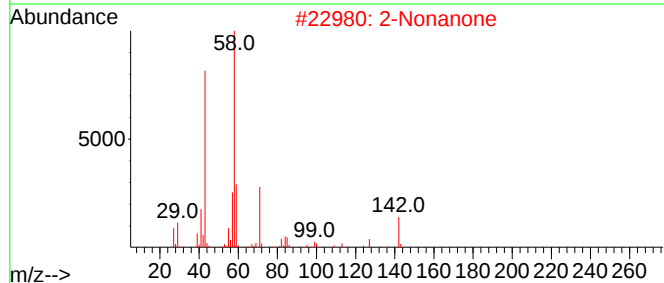
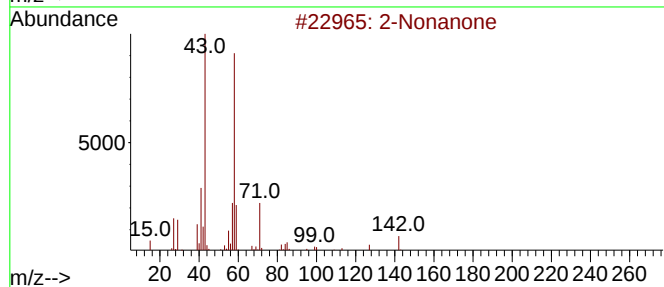
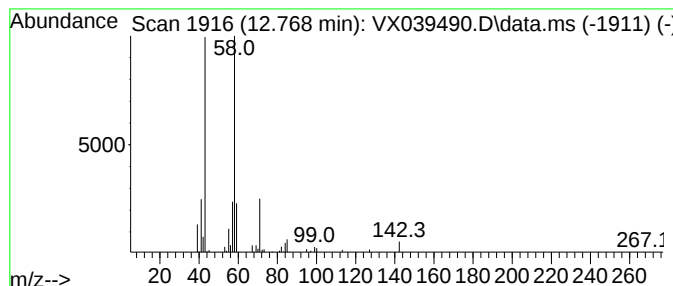
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Quant Title : VOC Analysis

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

Peak Number 15 2-Nonanone Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.768	3.16 ug/L	40678	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonanone			142	C9H18O	000821-55-6	91
2	2-Nonanone			142	C9H18O	000821-55-6	91
3	2-Nonanone			142	C9H18O	000821-55-6	91
4	2-Undecanone			170	C11H22O	000112-12-9	78
5	2-Dodecanone			184	C12H24O	006175-49-1	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122723\
Data File : VX039490.D
Acq On : 27 Dec 2023 12:43
Operator : JC/MD
Sample : 05989-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
F7A62

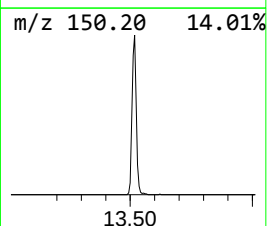
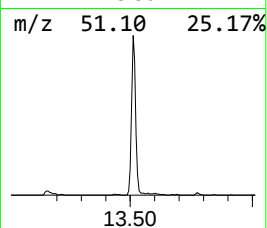
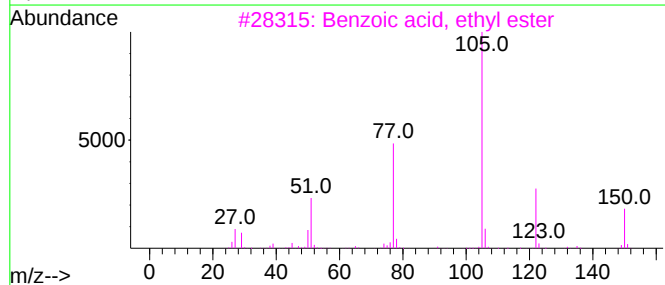
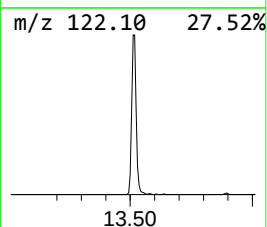
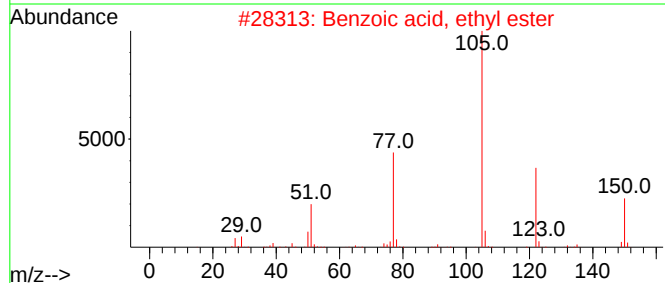
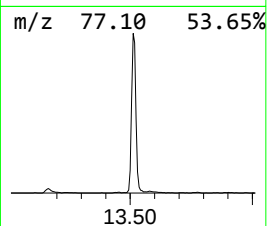
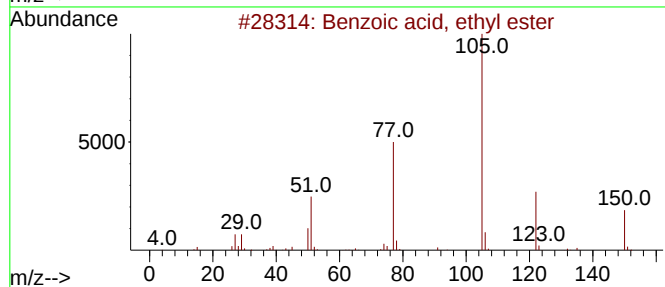
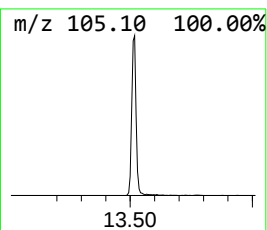
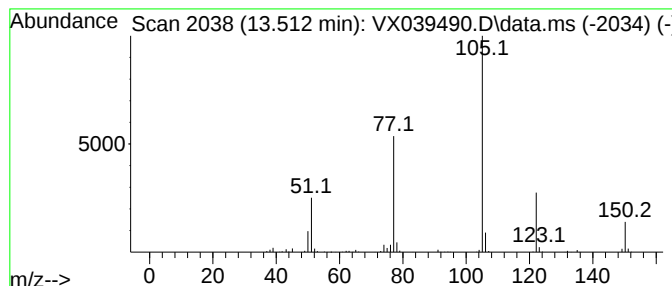
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Quant Title : VOC Analysis

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

Peak Number 16 Benzoic acid, ethyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.512	19.79 ug/L	255034	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	95
2			Benzoic acid, ethyl ester	150	C9H10O2	000093-89-0	94
3			Benzoic acid, ethyl ester	150	C9H10O2	000093-89-0	94
4			Benzoic acid, ethyl ester	150	C9H10O2	000093-89-0	91
5			Butanedioic acid, 2,3-bis(benzoy...	358	C18H14O8	002743-38-6	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122723\
 Data File : VX039490.D
 Acq On : 27 Dec 2023 12:43
 Operator : JC/MD
 Sample : 05989-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 F7A62

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

TIC Library : C:\Database\NIST0.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Isopropyl Alcohol	2.532	10.2	ug/L	106324	1	6.763	521244	50.0
2-Butanol	4.989	47.6	ug/L	495904	1	6.763	521244	50.0
1-Butanol	7.208	11.9	ug/L	123893	1	6.763	521244	50.0
2-Pentanone	7.452	17.7	ug/L	184441	1	6.763	521244	50.0
3-Pentanone	7.641	3.9	ug/L	40264	1	6.763	521244	50.0
2-Pentanol	7.903	6.4	ug/L	66555	1	6.763	521244	50.0
1-Hexanol	10.579	3.5	ug/L	44629	2	10.055	643396	50.0
2-Heptanone	10.769	29.3	ug/L	376458	2	10.055	643396	50.0
2-Heptanol	10.878	11.4	ug/L	147100	2	10.055	643396	50.0
3-Octanone	11.756	166.0	ug/L	2138410	3	12.024	644256	50.0
3-Octanol	11.848	86.8	ug/L	1118680	3	12.024	644256	50.0
2-Octanol, (S)-	11.896	9.9	ug/L	127811	3	12.024	644256	50.0
2-Nonanone	12.768	3.2	ug/L	40678	3	12.024	644256	50.0
Benzoic acid, e...	13.512	19.8	ug/L	255034	3	12.024	644256	50.0