

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122723\
 Data File : VX039498.D
 Acq On : 27 Dec 2023 15:44
 Operator : JC/MD
 Sample : 05989-03DL 4X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 F7A62DL

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: VX039498.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	32	rBV2	6550	13952	1.96%	0.194%
2	1.368	42	46	56	rBV	72715	76129	10.68%	1.057%
3	1.453	57	60	63	rVV	5467	5601	0.79%	0.078%
4	1.666	91	95	107	rVB	55173	79455	11.14%	1.103%
5	2.057	156	159	167	rVB	6100	9505	1.33%	0.132%
6	2.307	194	200	207	rBV	138505	213982	30.01%	2.970%
7	2.380	207	212	216	rVV	32011	52865	7.42%	0.734%
8	2.416	216	218	228	rVB	13721	22440	3.15%	0.311%
9	2.532	230	237	246	rBV	12972	25371	3.56%	0.352%
10	2.703	262	265	270	rVB	1110	1359	0.19%	0.019%
11	2.782	275	278	284	rVV4	1244	2147	0.30%	0.030%
12	2.947	298	305	314	rVB	7502	17236	2.42%	0.239%
13	3.105	329	331	335	rVB	308	281	0.04%	0.004%
14	3.331	364	368	369	rBV2	309	329	0.05%	0.005%
15	3.867	451	456	459	rBV3	700	1321	0.19%	0.018%
16	4.257	513	520	524	rVB5	614	1404	0.20%	0.019%
17	4.300	524	527	529	rBV2	282	332	0.05%	0.005%
18	4.367	531	538	539	rBV2	311	500	0.07%	0.007%
19	4.452	543	552	562	rBV	96847	288105	40.41%	3.999%
20	4.556	562	569	589	rVV	95650	277099	38.87%	3.847%
21	4.715	593	595	601	rVB2	559	542	0.08%	0.008%
22	4.995	632	641	644	rBV2	34502	85140	11.94%	1.182%
23	5.391	704	706	708	rBV3	527	514	0.07%	0.007%
24	5.550	728	732	734	rBV2	343	525	0.07%	0.007%
25	5.684	751	754	756	rBV2	250	317	0.04%	0.004%
26	5.971	788	801	820	rBV2	237856	712936	100.00%	9.897%
27	6.117	824	825	827	rBV2	886	660	0.09%	0.009%
28	6.647	907	912	915	rVV3	338	576	0.08%	0.008%
29	6.763	922	931	944	rBV	204701	497554	69.79%	6.907%
30	6.946	960	961	966	rVB2	415	392	0.05%	0.005%
31	6.983	966	967	970	rBV	248	282	0.04%	0.004%
32	7.214	999	1005	1012	rBV2	10939	24062	3.38%	0.334%
33	7.306	1013	1020	1031	rVB	154991	336653	47.22%	4.673%
34	7.458	1039	1045	1059	rBV	18080	39210	5.50%	0.544%
35	7.647	1071	1076	1082	rBV2	3130	5981	0.84%	0.083%
36	7.909	1113	1119	1130	rBV3	4384	12810	1.80%	0.178%

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Integrator: RTE

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 Title : VOC Analysis

37	8.324	1180	1187	1203	rBV	97158	164343	23.05%	2.281%
38	8.452	1206	1208	1210	rBV3	238	293	0.04%	0.004%
39	8.494	1213	1215	1217	rBV	576	644	0.09%	0.009%
40	8.580	1224	1229	1234	rBV2	4653	8039	1.13%	0.112%
41	8.647	1234	1240	1250	rBV	341651	537835	75.44%	7.466%
42	8.952	1284	1290	1301	rVV	69544	107431	15.07%	1.491%
43	9.244	1333	1338	1341	rBV2	1259	2138	0.30%	0.030%
44	9.342	1350	1354	1356	rBV2	3428	4123	0.58%	0.057%
45	9.385	1356	1361	1368	rBV	412382	588177	82.50%	8.165%
46	9.525	1381	1384	1392	rVB4	3057	4463	0.63%	0.062%
47	10.055	1465	1471	1486	rBV	437353	614324	86.17%	8.528%
48	10.366	1518	1522	1526	rVB2	248	357	0.05%	0.005%
49	10.409	1526	1529	1533	rBV3	379	542	0.08%	0.008%
50	10.586	1553	1558	1565	rBV	4611	8222	1.15%	0.114%
51	10.768	1583	1588	1600	rBV	55797	75830	10.64%	1.053%
52	10.878	1602	1606	1618	rBV	16725	28937	4.06%	0.402%
53	11.085	1637	1640	1645	rVB3	1746	2208	0.31%	0.031%
54	11.189	1652	1657	1671	rVB	328682	416070	58.36%	5.776%
55	11.378	1686	1688	1689	rBV	436	282	0.04%	0.004%
56	11.427	1693	1696	1700	rBV4	816	1195	0.17%	0.017%
57	11.683	1736	1738	1740	rBV2	1048	1270	0.18%	0.018%
58	11.756	1745	1750	1760	rBV	359999	433403	60.79%	6.016%
59	11.848	1760	1765	1771	rBV2	131134	190273	26.69%	2.641%
60	12.018	1788	1793	1802	rVB	470406	602387	84.49%	8.362%
61	12.140	1811	1813	1820	rVB4	3389	4743	0.67%	0.066%
62	12.219	1822	1826	1831	rBV3	3619	5437	0.76%	0.075%
63	12.317	1837	1842	1849	rBV	416923	514342	72.14%	7.140%
64	12.561	1880	1882	1886	rBV3	1141	1251	0.18%	0.017%
65	12.695	1901	1904	1908	rVB4	1111	1543	0.22%	0.021%
66	12.768	1911	1916	1919	rBV	5382	7530	1.06%	0.105%
67	12.988	1949	1952	1954	rBV3	296	397	0.06%	0.006%
68	13.097	1967	1970	1972	rBV2	342	369	0.05%	0.005%
69	13.164	1978	1981	1991	rVV5	1820	3400	0.48%	0.047%
70	13.298	2001	2003	2008	rVB2	463	496	0.07%	0.007%
71	13.408	2018	2021	2023	rBV	410	470	0.07%	0.007%
72	13.445	2024	2027	2034	rVB2	1220	1781	0.25%	0.025%
73	13.518	2034	2039	2046	rBV	40352	49678	6.97%	0.690%
74	13.676	2063	2065	2067	rBV	343	367	0.05%	0.005%
75	13.774	2076	2081	2085	rVB3	795	1178	0.17%	0.016%
76	13.823	2088	2089	2095	rVB2	349	305	0.04%	0.004%

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Stop Thrs : 0

Peak Location: TOP

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 Title : VOC Analysis

77	13.884	2095	2099	2102	rBV3	344	506	0.07%	0.007%
78	14.073	2126	2130	2133	rVB2	327	368	0.05%	0.005%
79	14.121	2136	2138	2141	rBV3	421	378	0.05%	0.005%
80	14.152	2141	2143	2147	rVB2	312	378	0.05%	0.005%
81	14.207	2150	2152	2157	rVB3	254	287	0.04%	0.004%
82	14.268	2157	2162	2163	rBV	246	313	0.04%	0.004%
83	14.304	2164	2168	2170	rVB3	768	766	0.11%	0.011%
84	14.371	2176	2179	2182	rBV3	455	462	0.06%	0.006%
85	14.506	2199	2201	2204	rBV4	734	821	0.12%	0.011%
86	14.603	2214	2217	2220	rBV3	263	303	0.04%	0.004%
87	14.640	2220	2223	2227	rBV3	579	804	0.11%	0.011%
88	14.780	2244	2246	2249	rVB3	428	430	0.06%	0.006%
89	15.060	2289	2292	2293	rBV2	445	360	0.05%	0.005%
90	15.121	2299	2302	2304	rBV2	394	399	0.06%	0.006%
91	15.194	2312	2314	2316	rBV2	364	386	0.05%	0.005%
92	15.237	2318	2321	2324	rBV2	213	343	0.05%	0.005%
93	15.359	2340	2341	2344	rVB2	332	292	0.04%	0.004%
94	15.627	2384	2385	2388	rBV2	337	338	0.05%	0.005%
95	15.835	2418	2419	2422	rVB2	426	292	0.04%	0.004%
96	15.908	2426	2431	2434	rBV3	324	531	0.07%	0.007%
97	16.036	2447	2452	2455	rBV2	260	488	0.07%	0.007%
98	16.164	2469	2473	2477	rBV3	261	428	0.06%	0.006%
99	16.200	2477	2479	2481	rVB2	397	312	0.04%	0.004%
100	16.731	2563	2566	2567	rBV2	304	268	0.04%	0.004%

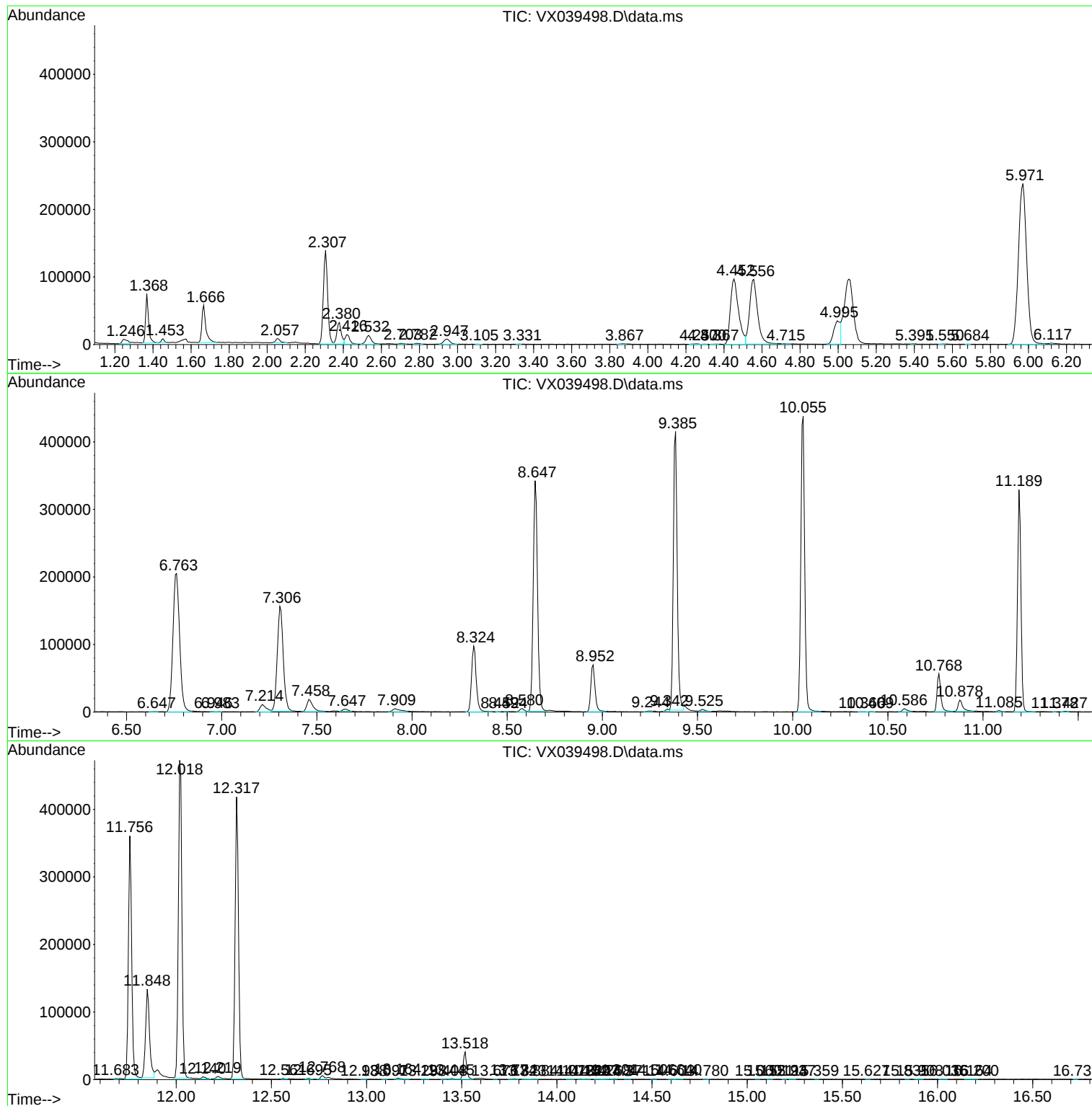
Sum of corrected areas: 7203893

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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



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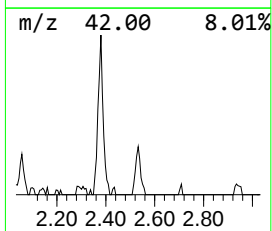
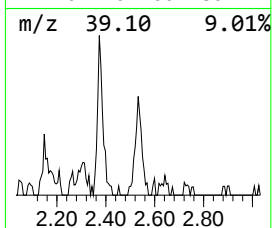
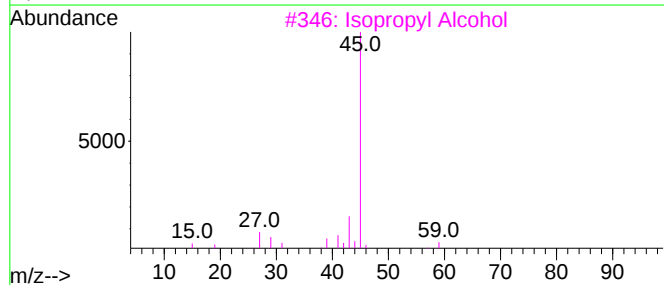
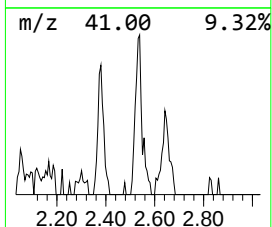
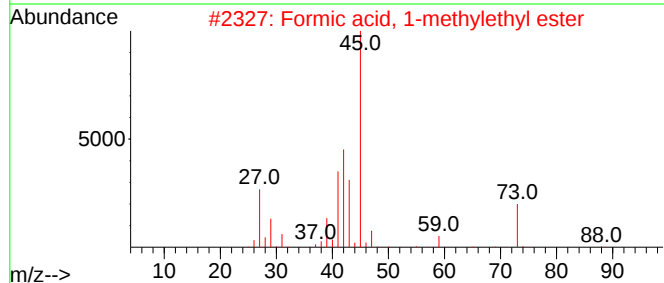
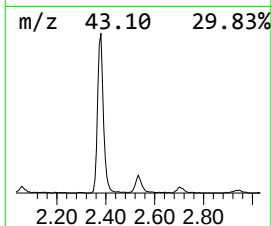
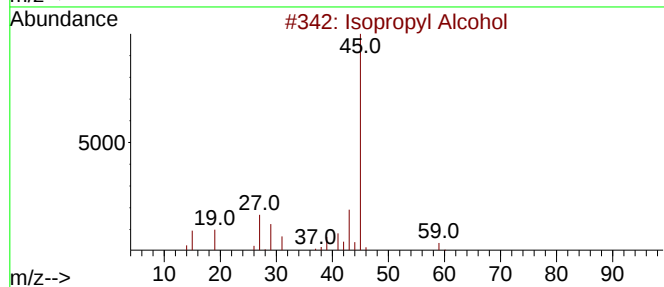
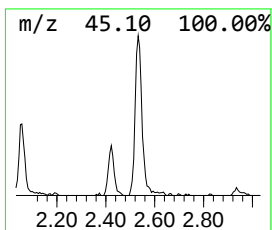
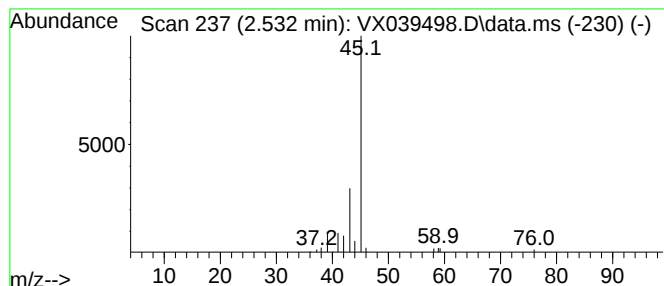
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.532	2.55 ug/L	25371	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	43
2			Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	40
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5			Isopropyl Alcohol	60	C3H8O	000067-63-0	9



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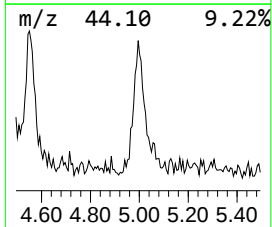
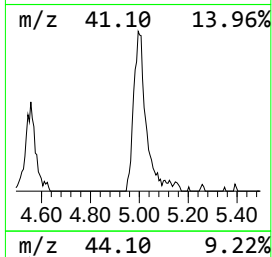
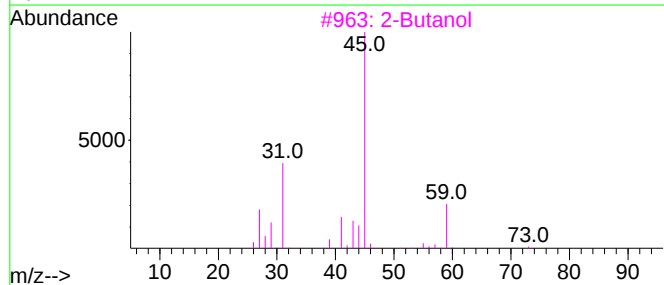
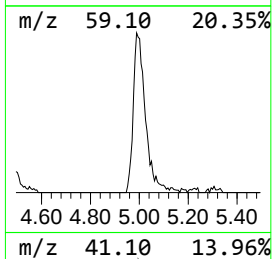
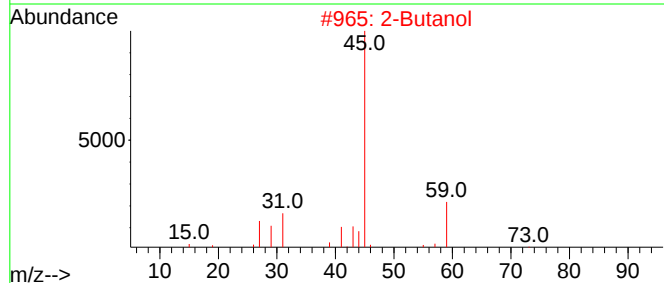
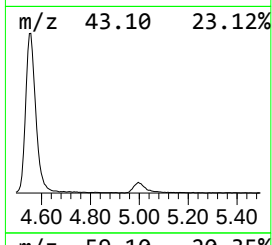
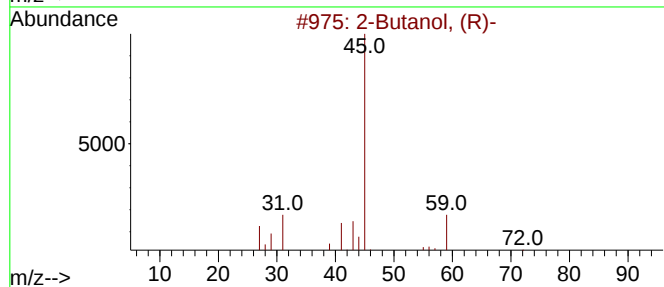
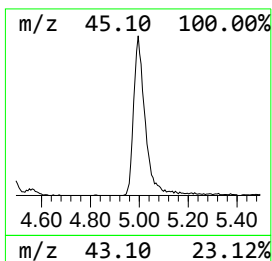
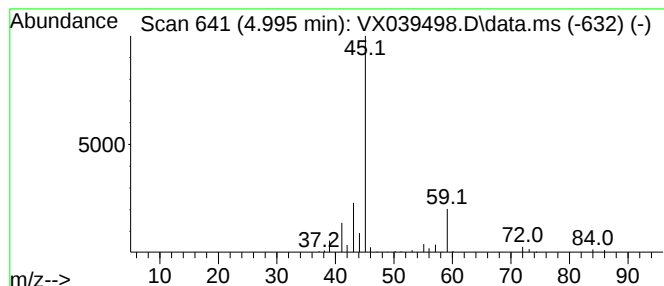
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 2-Butanol, (R)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.995	8.56 ug/L	85140	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, (R)-			74	C4H10O	014898-79-4	83
2	2-Butanol			74	C4H10O	000078-92-2	83
3	2-Butanol			74	C4H10O	000078-92-2	78
4	2-Butanol, (R)-			74	C4H10O	014898-79-4	74
5	2-Butanol			74	C4H10O	000078-92-2	72



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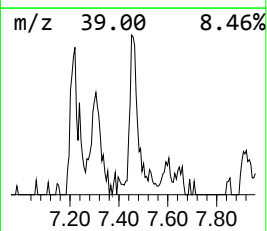
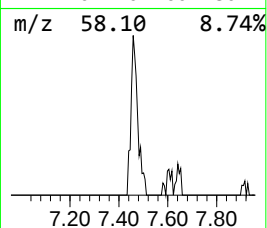
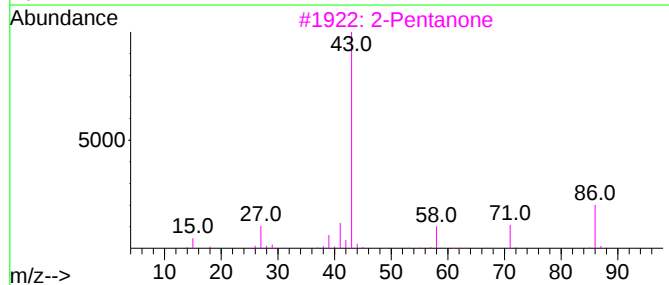
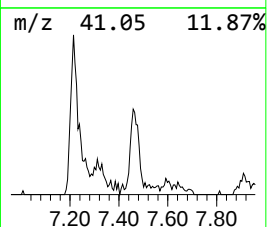
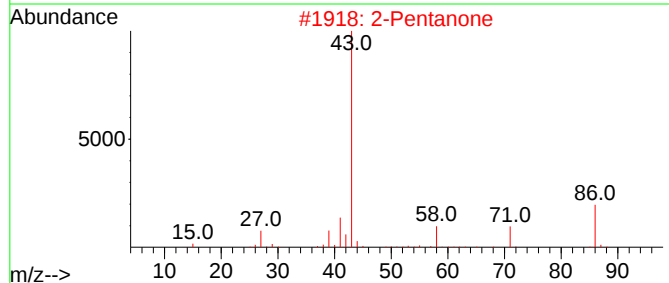
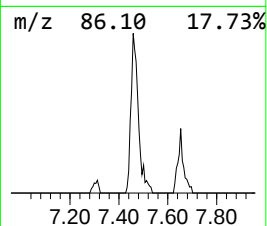
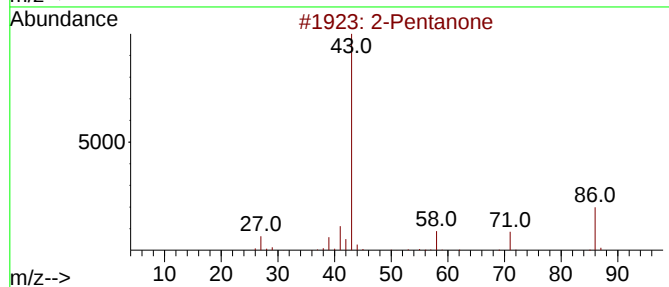
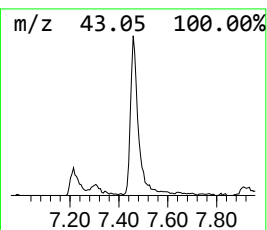
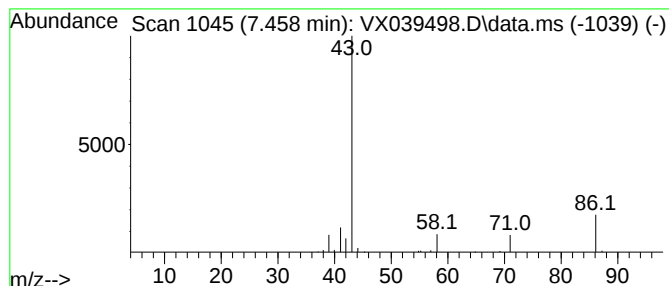
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 2-Pentanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.458	3.94 ug/L	39210	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone			86	C5H10O	000107-87-9	80
2	2-Pentanone			86	C5H10O	000107-87-9	80
3	2-Pentanone			86	C5H10O	000107-87-9	64
4	2-Pentanone			86	C5H10O	000107-87-9	64
5	2,3-Butanedione			86	C4H6O2	000431-03-8	59



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Acq On : 27 Dec 2023 15:44
Operator : JC/MD
Sample : 05989-03DL 4X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
F7A62DL

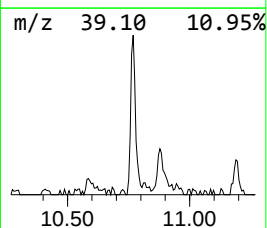
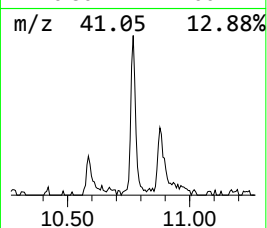
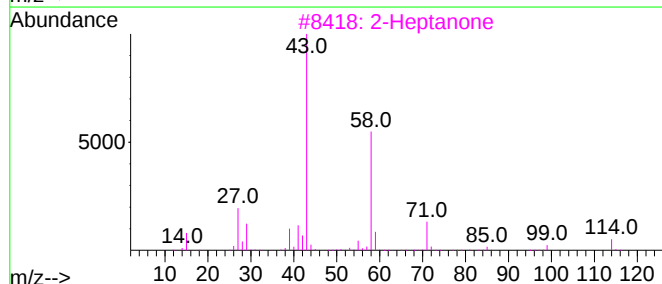
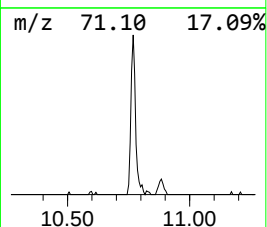
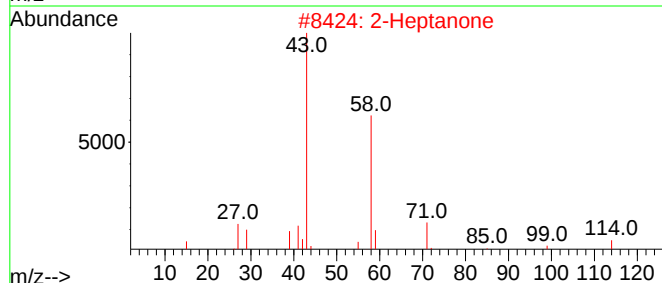
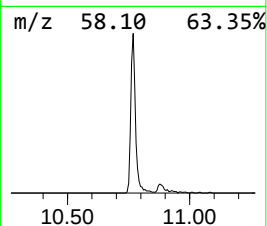
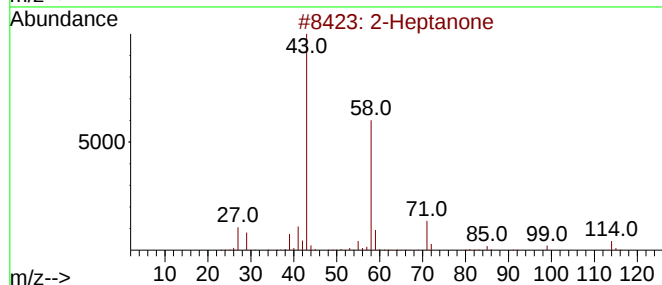
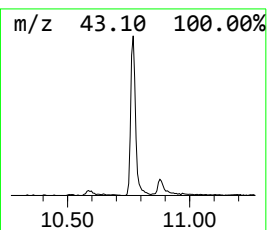
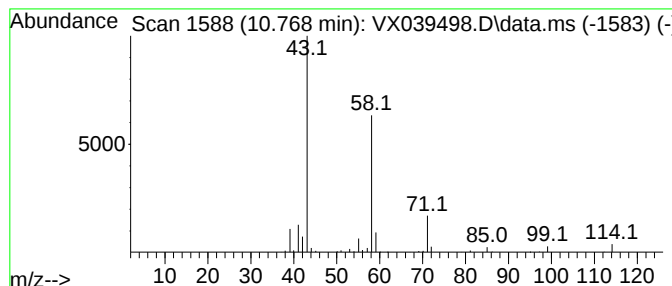
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Quant Title : VOC Analysis

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

Peak Number 5 2-Heptanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.768	6.17 ug/L	75830	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	90
3	2-Heptanone			114	C7H14O	000110-43-0	90
4	2-Heptanone			114	C7H14O	000110-43-0	90
5	2-Heptanone			114	C7H14O	000110-43-0	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122723\
Data File : VX039498.D
Acq On : 27 Dec 2023 15:44
Operator : JC/MD
Sample : 05989-03DL 4X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
F7A62DL

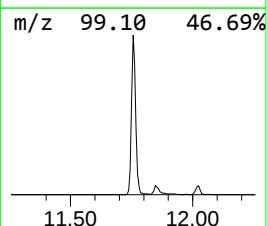
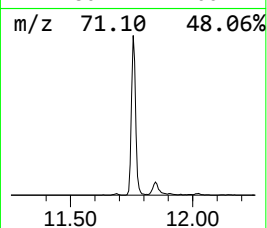
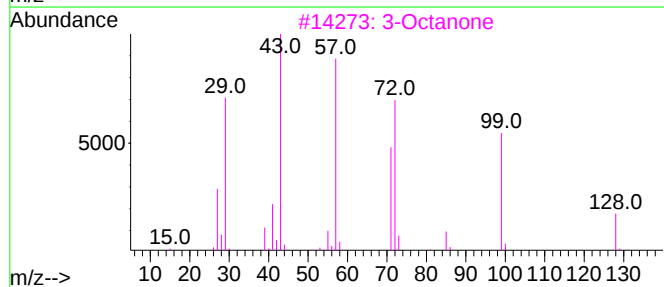
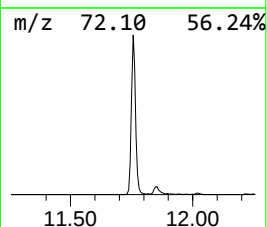
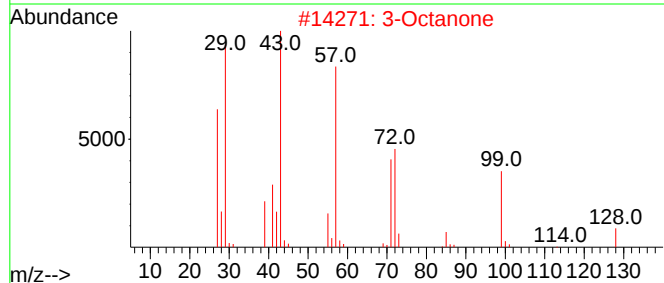
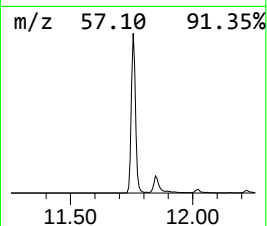
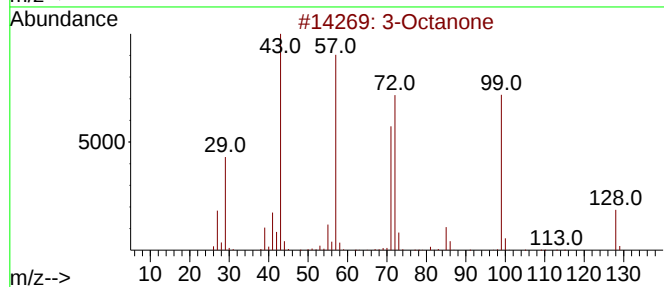
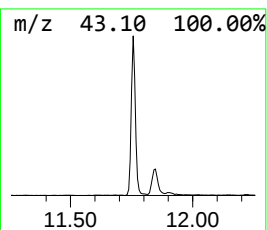
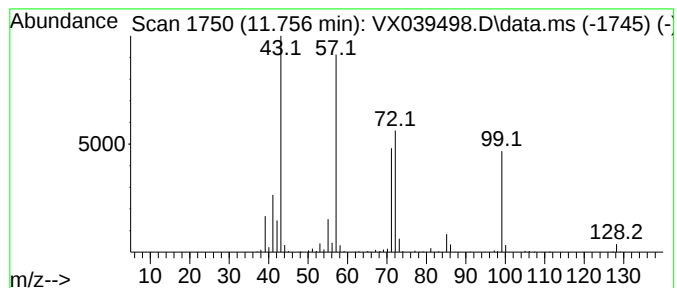
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Quant Title : VOC Analysis

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

Peak Number 6 3-Octanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.756	35.97 ug/L	433403	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	74
3	3-Octanone			128	C8H16O	000106-68-3	53
4	Ethanone, 1-(3,3-dimethyloxiranyl)-			114	C6H10O2	004478-63-1	50
5	3-Heptanone, 5-methyl-			128	C8H16O	000541-85-5	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122723\
Data File : VX039498.D
Acq On : 27 Dec 2023 15:44
Operator : JC/MD
Sample : 05989-03DL 4X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
F7A62DL

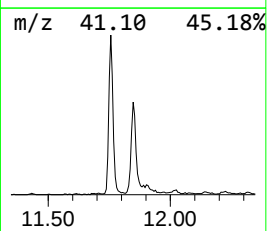
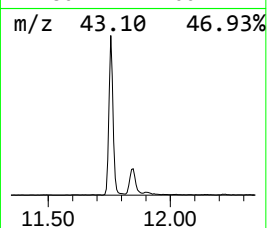
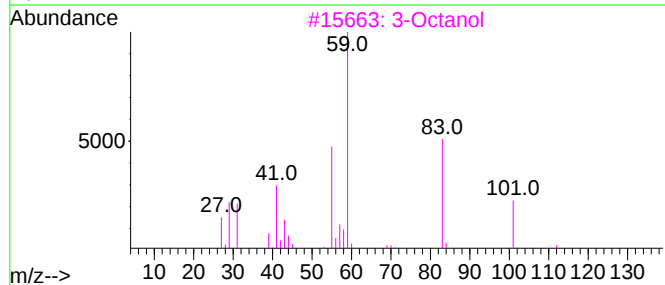
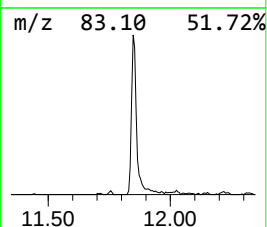
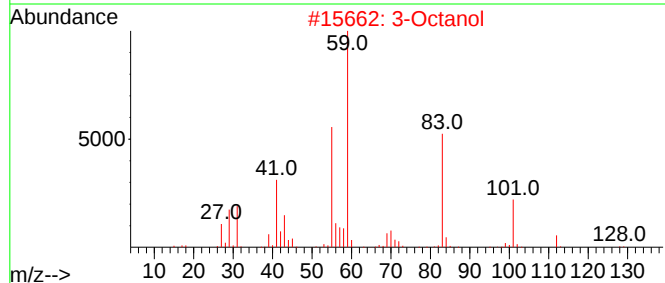
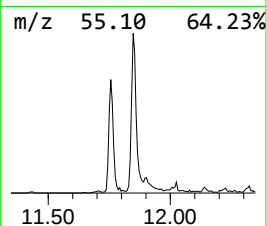
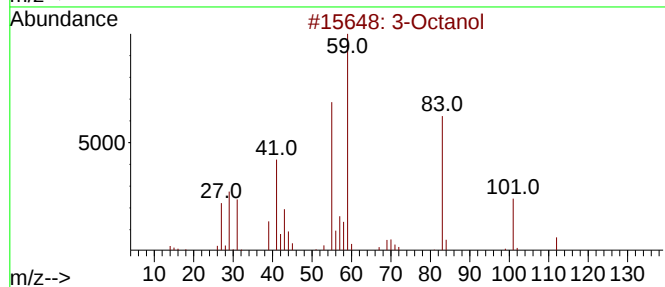
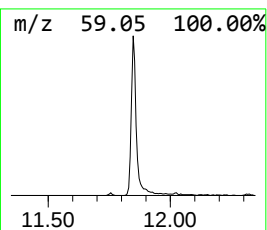
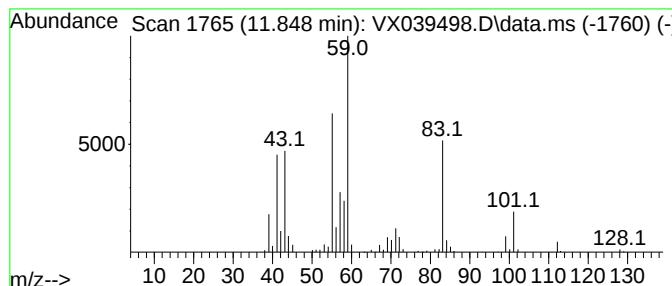
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Quant Title : VOC Analysis

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

Peak Number 7 3-Octanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.848	15.79 ug/L	190273	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-Heptanol, 6-methyl-	130	C8H18O	018720-66-6	59
5			3-Heptanol, 6-methyl-	130	C8H18O	018720-66-6	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122723\
Data File : VX039498.D
Acq On : 27 Dec 2023 15:44
Operator : JC/MD
Sample : 05989-03DL 4X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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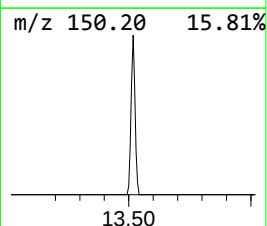
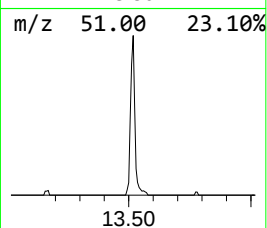
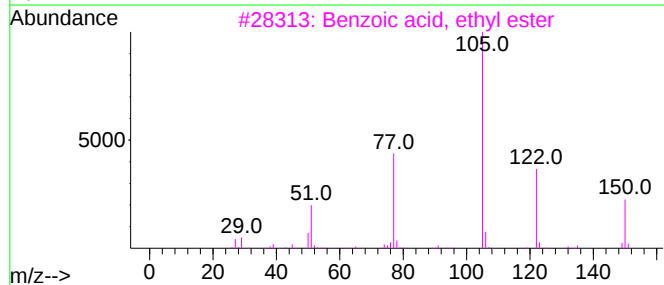
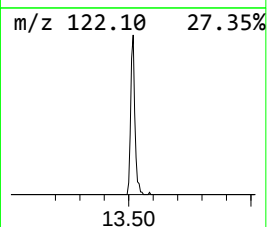
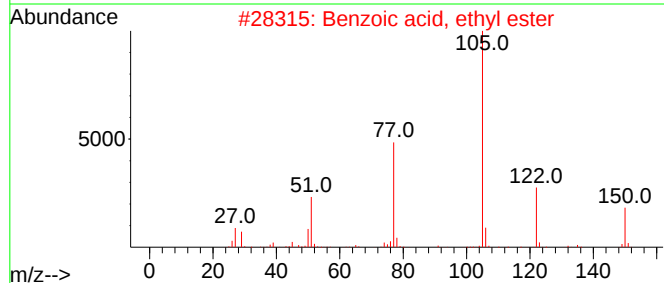
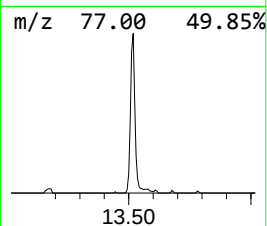
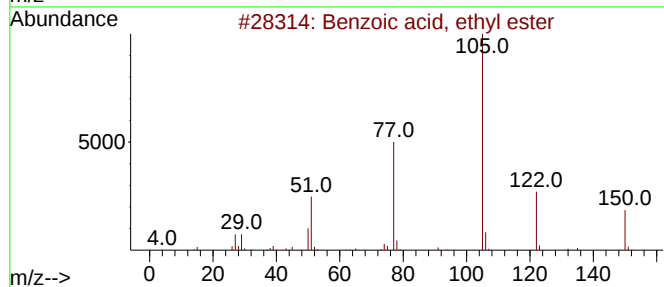
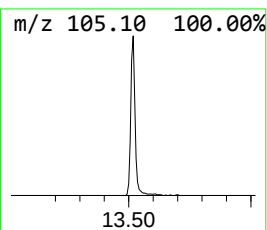
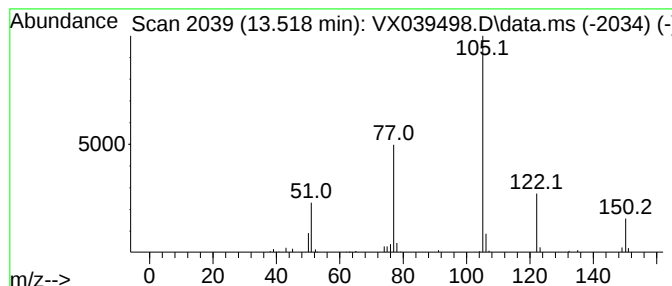
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Quant Title : VOC Analysis

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

Peak Number 8 Benzoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.518	4.12 ug/L	49678	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	91
4			Benzoic acid, ethyl ester	150	C9H10O2	000093-89-0	91
5			Octanediamide, N,N'-di-benzoyloxy-	412	C22H24N2O6	1000253-26-1	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122723\
Data File : VX039498.D
Acq On : 27 Dec 2023 15:44
Operator : JC/MD
Sample : 05989-03DL 4X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
F7A62DL

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
unknown-01	2.532	2.5	ug/L	25371	1	6.763	497554	50.0
2-Butanol, (R)-	4.995	8.6	ug/L	85140	1	6.763	497554	50.0
2-Pentanone	7.458	3.9	ug/L	39210	1	6.763	497554	50.0
2-Heptanone	10.768	6.2	ug/L	75830	2	10.055	614324	50.0
3-Octanone	11.756	36.0	ug/L	433403	3	12.024	602387	50.0
3-Octanol	11.848	15.8	ug/L	190273	3	12.024	602387	50.0
Benzoic acid, e...	13.518	4.1	ug/L	49678	3	12.024	602387	50.0