

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121724\
 Data File : VX044353.D
 Acq On : 17 Dec 2024 15:48
 Operator : JC/MD
 Sample : P5235-14 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AX6

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120524WMA.M
 Title : VOC Analysis

Signal : TIC: VX044353.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	7	9	12	rVB3	2788	2374	0.23%	0.029%
2	1.367	43	46	56	rVB	117949	131096	12.87%	1.585%
3	1.453	57	60	65	rVB	7710	9158	0.90%	0.111%
4	1.648	89	92	99	rVB	104172	138513	13.59%	1.674%
5	2.300	193	199	208	rBV	190860	297328	29.18%	3.594%
6	2.385	209	213	224	rVB	25898	42817	4.20%	0.518%
7	2.562	238	242	245	rBV3	1924	2764	0.27%	0.033%
8	2.715	263	267	272	rVB4	1972	3860	0.38%	0.047%
9	2.788	272	279	284	rBV5	2099	4436	0.44%	0.054%
10	2.946	296	305	316	rBV	17021	41787	4.10%	0.505%
11	3.263	355	357	358	rVB	945	595	0.06%	0.007%
12	3.434	379	385	387	rBV3	1506	2865	0.28%	0.035%
13	3.593	405	411	421	rVV4	3088	9113	0.89%	0.110%
14	3.989	475	476	480	rBV2	490	631	0.06%	0.008%
15	4.031	480	483	486	rBV2	589	915	0.09%	0.011%
16	4.257	518	520	522	rVV2	885	944	0.09%	0.011%
17	4.464	546	554	570	rVV	73867	220315	21.62%	2.663%
18	5.062	640	652	665	rBV	137578	428817	42.08%	5.183%
19	5.574	734	736	740	rBV3	888	907	0.09%	0.011%
20	5.684	750	754	756	rBV2	460	698	0.07%	0.008%
21	5.970	789	801	825	rBV2	342278	1018964	100.00%	12.316%
22	6.281	850	852	854	rBV3	690	813	0.08%	0.010%
23	6.360	858	865	876	rVB2	7691	22087	2.17%	0.267%
24	6.501	885	888	891	rVB2	740	830	0.08%	0.010%
25	6.763	922	931	944	rBV	251360	612097	60.07%	7.398%
26	7.000	969	970	976	rBV3	751	858	0.08%	0.010%
27	7.116	985	989	990	rBV4	1668	2162	0.21%	0.026%
28	7.305	1012	1020	1035	rVV	207645	475023	46.62%	5.742%
29	7.598	1064	1068	1069	rBV	2055	2450	0.24%	0.030%
30	7.805	1096	1102	1121	rBV	105139	199095	19.54%	2.406%
31	8.110	1149	1152	1154	rBV2	605	638	0.06%	0.008%
32	8.232	1168	1172	1173	rBV2	756	651	0.06%	0.008%
33	8.323	1181	1187	1200	rBV	125302	212682	20.87%	2.571%
34	8.549	1218	1224	1234	rBV	22919	43604	4.28%	0.527%
35	8.647	1234	1240	1251	rBV	485016	758657	74.45%	9.170%
36	8.951	1285	1290	1303	rBV2	110776	176934	17.36%	2.139%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
 Title : VOC Analysis

37	9.244	1334	1338	1346	rVB	27304	42192	4.14%	0.510%
38	9.342	1348	1354	1356	rBV4	5236	8441	0.83%	0.102%
39	9.384	1356	1361	1373	rVV	325816	480090	47.12%	5.803%
40	9.488	1374	1378	1382	rBV	44733	60495	5.94%	0.731%
41	9.585	1390	1394	1404	rVB	30284	44246	4.34%	0.535%
42	9.695	1410	1412	1417	rBV5	1474	1610	0.16%	0.019%
43	9.915	1443	1448	1456	rBV	88379	116459	11.43%	1.408%
44	9.994	1459	1461	1463	rVB2	1275	903	0.09%	0.011%
45	10.055	1465	1471	1481	rBV	518113	726913	71.34%	8.786%
46	10.195	1491	1494	1500	rVB3	5270	7166	0.70%	0.087%
47	10.256	1500	1504	1505	rVB3	538	640	0.06%	0.008%
48	10.299	1507	1511	1519	rVB2	16071	24960	2.45%	0.302%
49	10.433	1530	1533	1535	rVB3	556	614	0.06%	0.007%
50	10.463	1535	1538	1540	rBV2	632	810	0.08%	0.010%
51	10.518	1543	1547	1548	rBV	1010	1252	0.12%	0.015%
52	10.640	1563	1567	1578	rVB	28719	42753	4.20%	0.517%
53	10.780	1588	1590	1592	rBV2	873	800	0.08%	0.010%
54	10.957	1618	1619	1623	rVB2	967	1048	0.10%	0.013%
55	11.189	1652	1657	1668	rVB	382740	501007	49.17%	6.056%
56	11.378	1686	1688	1696	rVB3	2078	3203	0.31%	0.039%
57	11.451	1697	1700	1704	rVB2	3713	4008	0.39%	0.048%
58	11.573	1717	1720	1725	rBV4	672	1326	0.13%	0.016%
59	11.616	1725	1727	1730	rVV3	1591	1673	0.16%	0.020%
60	11.756	1745	1750	1757	rBV4	5793	9687	0.95%	0.117%
61	11.841	1762	1764	1767	rBV4	954	1142	0.11%	0.014%
62	11.963	1781	1784	1788	rVB3	3670	5037	0.49%	0.061%
63	12.018	1788	1793	1802	rBV	455161	591901	58.09%	7.154%
64	12.091	1802	1805	1813	rVB6	6095	10352	1.02%	0.125%
65	12.189	1819	1821	1824	rVB3	759	667	0.07%	0.008%
66	12.243	1826	1830	1834	rVV3	2181	3378	0.33%	0.041%
67	12.317	1837	1842	1853	rVV	487968	627335	61.57%	7.583%
68	12.390	1853	1854	1861	rVB5	1796	2035	0.20%	0.025%
69	12.524	1873	1876	1879	rBV3	1048	1389	0.14%	0.017%
70	12.609	1888	1890	1897	rBV5	782	1241	0.12%	0.015%
71	12.701	1903	1905	1908	rBV4	625	624	0.06%	0.008%
72	12.774	1914	1917	1922	rBV5	1733	2513	0.25%	0.030%
73	12.859	1927	1931	1934	rBV4	1528	2636	0.26%	0.032%
74	12.902	1934	1938	1944	rVV	12386	16946	1.66%	0.205%
75	12.963	1947	1948	1951	rVB2	1257	632	0.06%	0.008%
76	13.091	1965	1969	1972	rBV4	723	1136	0.11%	0.014%

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Integration Parameters: LSCINT.P

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 Title : VOC Analysis

77	13.164	1979	1981	1985	rVB2	1038	1053	0.10%	0.013%
78	13.292	1998	2002	2005	rBV5	1042	1650	0.16%	0.020%
79	13.335	2005	2009	2015	rVV5	5604	8541	0.84%	0.103%
80	13.426	2022	2024	2029	rVB3	1040	1246	0.12%	0.015%
81	13.505	2031	2037	2045	rVB5	8864	15154	1.49%	0.183%
82	13.731	2070	2074	2079	rBV6	985	1789	0.18%	0.022%
83	13.780	2079	2082	2087	rVV3	4087	5315	0.52%	0.064%
84	14.005	2115	2119	2121	rVV4	502	728	0.07%	0.009%
85	14.103	2131	2135	2137	rVV3	1896	2056	0.20%	0.025%
86	14.170	2144	2146	2148	rVB2	717	647	0.06%	0.008%
87	14.200	2148	2151	2154	rBV4	528	820	0.08%	0.010%
88	14.310	2167	2169	2170	rBV2	806	600	0.06%	0.007%
89	14.456	2186	2193	2195	rBV4	1679	2509	0.25%	0.030%
90	14.603	2216	2217	2219	rBV	918	600	0.06%	0.007%
91	14.639	2221	2223	2226	rBV3	1100	1501	0.15%	0.018%
92	14.786	2244	2247	2251	rVV4	1519	2414	0.24%	0.029%
93	15.072	2293	2294	2297	rBV4	625	639	0.06%	0.008%
94	15.115	2299	2301	2304	rBV2	859	1156	0.11%	0.014%
95	15.371	2340	2343	2344	rBV3	735	629	0.06%	0.008%
96	15.548	2368	2372	2375	rBV4	547	924	0.09%	0.011%
97	16.017	2444	2449	2451	rBV2	653	1141	0.11%	0.014%
98	16.054	2451	2455	2457	rVV3	823	1052	0.10%	0.013%
99	16.151	2467	2471	2476	rBV4	710	1739	0.17%	0.021%
100	16.548	2534	2536	2538	rBV3	842	785	0.08%	0.009%

Sum of corrected areas: 8273426

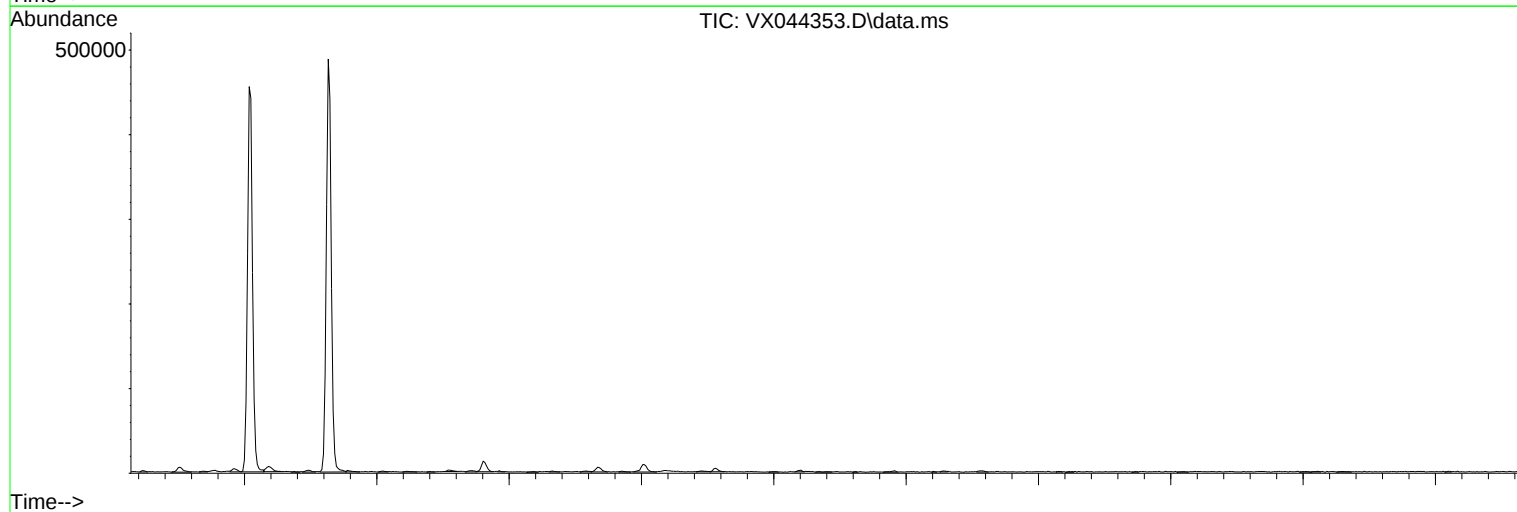
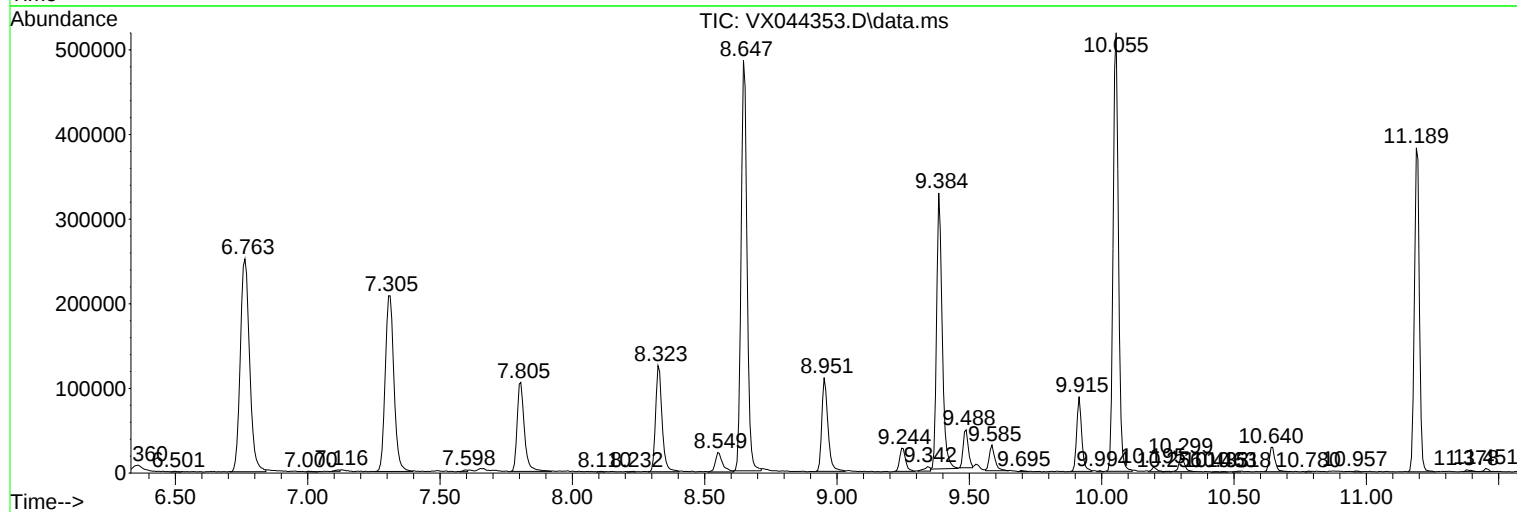
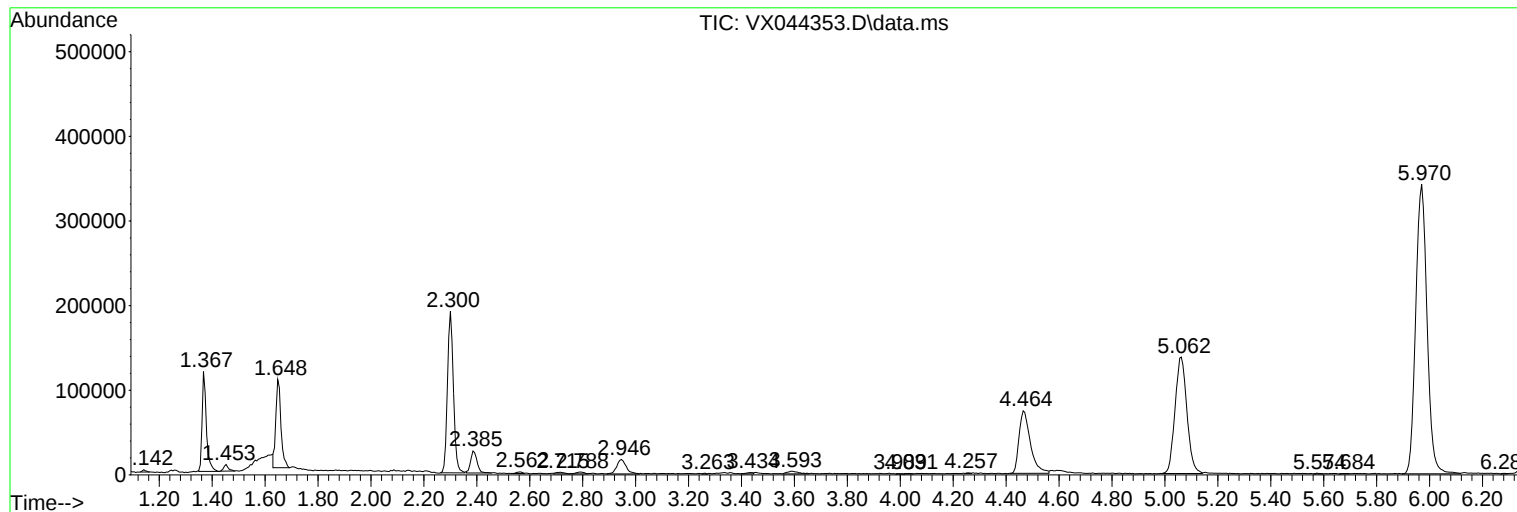
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Instrument :
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ClientSampleId :
C0AX6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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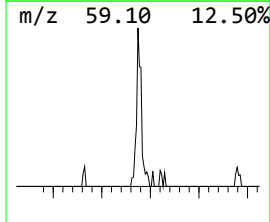
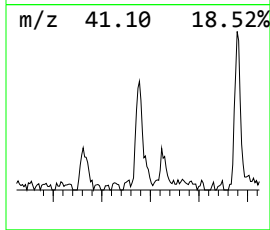
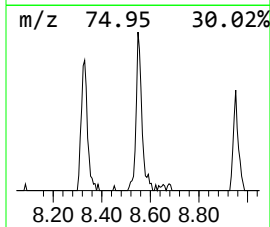
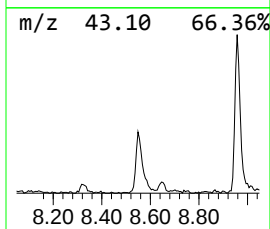
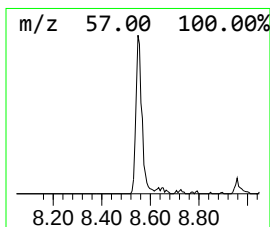
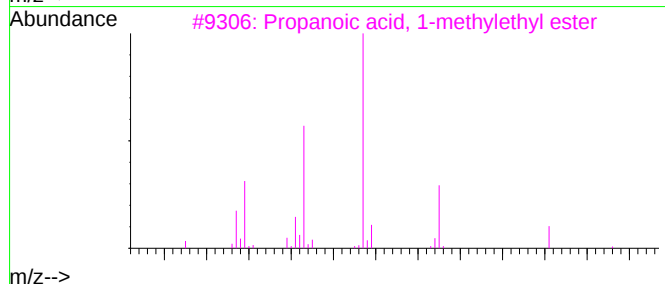
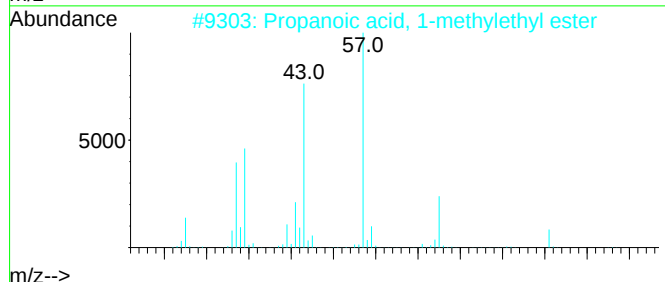
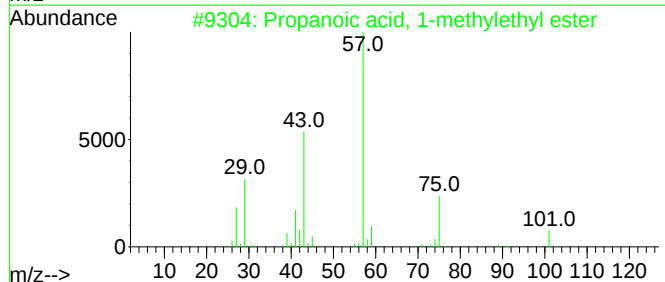
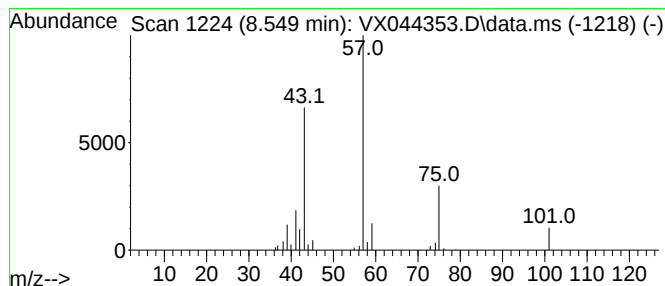
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 5 Propanoic acid, 1-methyleth... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.549	3.00 ug/L	43604	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	90
2	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
3	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	78
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	56
5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	50



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Quant Title : VOC Analysis

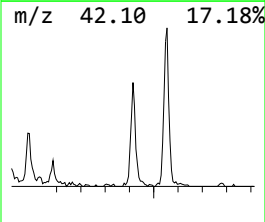
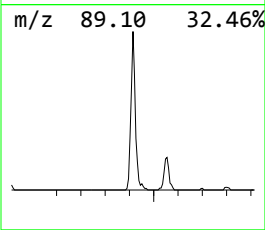
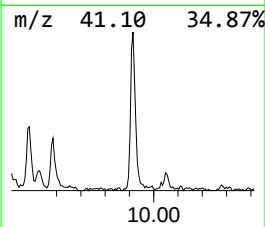
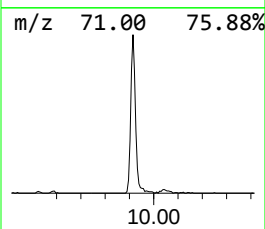
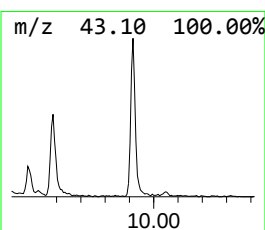
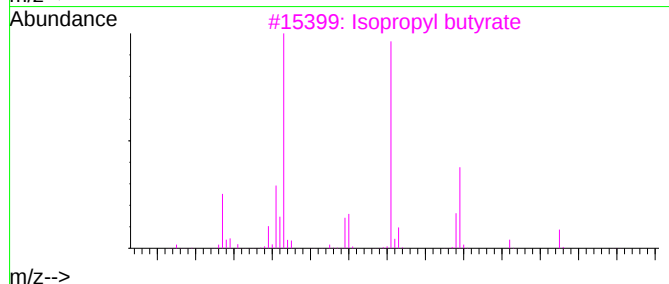
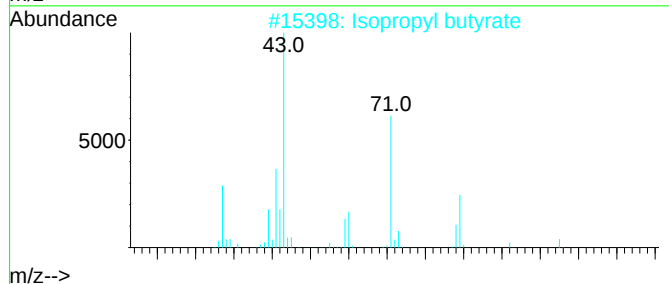
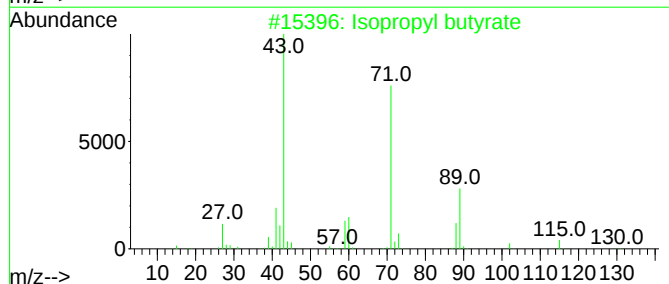
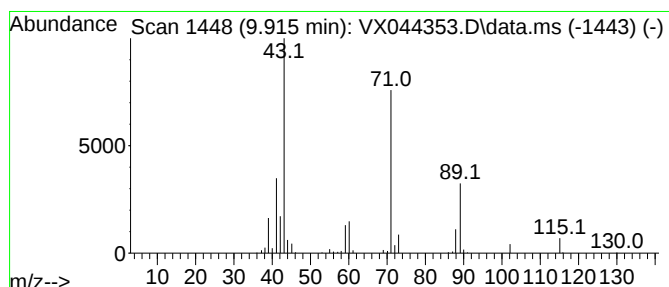
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 9 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	8.01 ug/L	116459	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	94
2	Isopropyl butyrate	130	C7H14O2	000638-11-9	90
3	Isopropyl butyrate	130	C7H14O2	000638-11-9	90
4	Isopropyl butyrate	130	C7H14O2	000638-11-9	83
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

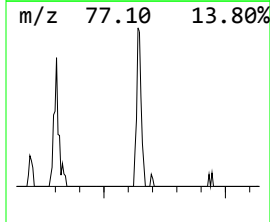
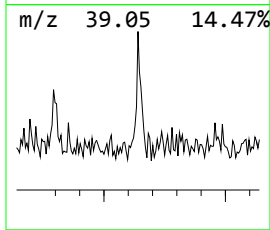
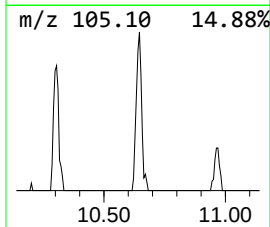
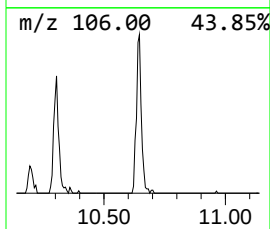
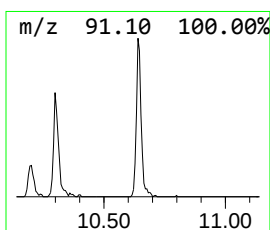
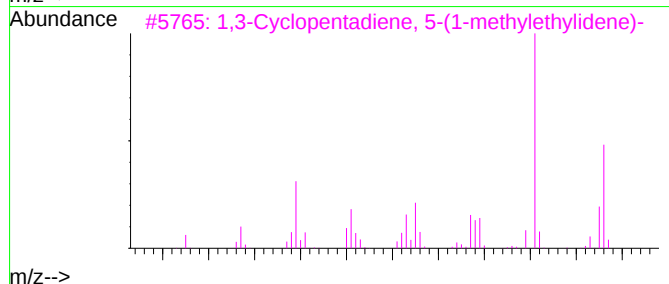
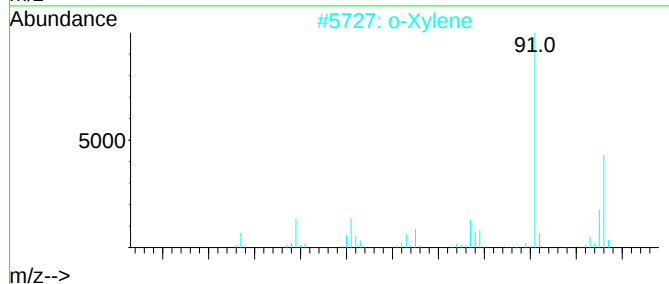
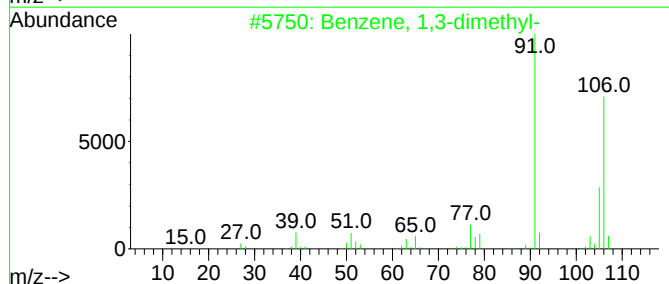
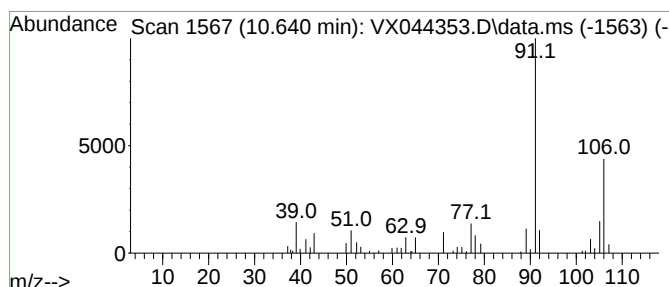
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 10 Benzene, 1,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.640	2.94 ug/L	42753	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	87
2	o-Xylene	106	C8H10	000095-47-6	87
3	1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	87
4	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	87
5	p-Xylene	106	C8H10	000106-42-3	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121724\
Data File : VX044353.D
Acq On : 17 Dec 2024 15:48
Operator : JC/MD
Sample : P5235-14 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0AX6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120524WMA.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
Propanoic acid,...	8.549	3.0	ug/L	43604	2	10.055	726913	50.0
Isopropyl butyrate	9.915	8.0	ug/L	116459	2	10.055	726913	50.0
Benzene, 1,3-di...	10.640	2.9	ug/L	42753	2	10.055	726913	50.0