

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122724\
 Data File : VX044519.D
 Acq On : 27 Dec 2024 14:35
 Operator : JC/MD
 Sample : P5326-06 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 YE685

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: VX044519.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.239	22	25	31	rBV4	3980	7314	0.73%	0.094%
2	1.367	43	46	56	rVB	118201	140222	14.03%	1.807%
3	1.642	88	91	104	rVB	95341	153486	15.36%	1.978%
4	2.294	192	198	208	rBV	216998	333374	33.37%	4.297%
5	2.385	209	213	218	rVB	4408	7594	0.76%	0.098%
6	2.574	240	244	247	rVV5	808	1326	0.13%	0.017%
7	2.782	274	278	284	rVB5	2384	3891	0.39%	0.050%
8	2.830	284	286	289	rBV4	582	517	0.05%	0.007%
9	2.940	296	304	313	rBV2	4341	11047	1.11%	0.142%
10	3.141	334	337	338	rBV2	571	653	0.07%	0.008%
11	3.434	380	385	394	rVV6	2801	6530	0.65%	0.084%
12	3.574	403	408	418	rBV3	3974	10268	1.03%	0.132%
13	3.855	453	454	459	rVB2	461	464	0.05%	0.006%
14	3.952	465	470	472	rBV4	395	737	0.07%	0.009%
15	3.989	474	476	478	rVB2	600	434	0.04%	0.006%
16	4.458	545	553	574	rBV	54427	181843	18.20%	2.344%
17	5.056	638	651	668	rVV3	134491	420688	42.10%	5.423%
18	5.263	683	685	687	rVB	800	665	0.07%	0.009%
19	5.403	704	708	710	rBV3	497	751	0.08%	0.010%
20	5.458	715	717	718	rBV	526	459	0.05%	0.006%
21	5.507	723	725	728	rVB3	535	515	0.05%	0.007%
22	5.543	728	731	732	rBV2	851	854	0.09%	0.011%
23	5.677	751	753	756	rVV2	414	447	0.04%	0.006%
24	5.964	789	800	816	rVV2	330420	999159	100.00%	12.879%
25	6.348	856	863	873	rBV2	6761	19073	1.91%	0.246%
26	6.488	885	886	890	rVB3	838	984	0.10%	0.013%
27	6.592	902	903	905	rBV2	474	438	0.04%	0.006%
28	6.635	908	910	914	rVV3	490	567	0.06%	0.007%
29	6.756	921	930	946	rBV	212404	512567	51.30%	6.607%
30	7.006	968	971	974	rBV3	574	868	0.09%	0.011%
31	7.128	983	991	996	rBV6	8617	21180	2.12%	0.273%
32	7.305	1011	1020	1034	rBV	199840	455537	45.59%	5.872%
33	7.653	1073	1077	1079	rBV2	3082	3589	0.36%	0.046%
34	7.799	1096	1101	1113	rBV	78533	147427	14.76%	1.900%
35	8.165	1158	1161	1162	rBV	644	515	0.05%	0.007%
36	8.323	1181	1187	1196	rBV	125528	201794	20.20%	2.601%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122724\
 Data File : VX044519.D
 Acq On : 27 Dec 2024 14:35
 Operator : JC/MD
 Sample : P5326-06 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 YE685

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\SFAMXLM120524WMA.M
 Title : VOC Analysis

37	8.439	1204	1206	1209	rBV3	494	448	0.04%	0.006%
38	8.549	1218	1224	1233	rBV	20394	36042	3.61%	0.465%
39	8.646	1233	1240	1251	rBV	476691	763085	76.37%	9.836%
40	8.860	1272	1275	1276	rBV3	621	499	0.05%	0.006%
41	8.951	1284	1290	1305	rVV2	94344	163975	16.41%	2.114%
42	9.244	1333	1338	1347	rBV	26942	43931	4.40%	0.566%
43	9.347	1347	1355	1356	rVV4	4884	8495	0.85%	0.110%
44	9.384	1356	1361	1372	rVV	264767	407739	40.81%	5.256%
45	9.488	1373	1378	1389	rVV	39464	66022	6.61%	0.851%
46	9.585	1390	1394	1404	rVB	22393	34511	3.45%	0.445%
47	9.914	1443	1448	1459	rBV	80064	112000	11.21%	1.444%
48	10.049	1465	1470	1479	rBV	413918	594934	59.54%	7.669%
49	10.305	1508	1512	1520	rVB7	2095	4845	0.48%	0.062%
50	10.463	1537	1538	1541	rVB2	1062	602	0.06%	0.008%
51	10.518	1541	1547	1548	rBV3	829	928	0.09%	0.012%
52	10.646	1563	1568	1576	rVB4	5733	8529	0.85%	0.110%
53	10.926	1610	1614	1617	rBV3	572	919	0.09%	0.012%
54	11.134	1645	1648	1650	rBV3	622	688	0.07%	0.009%
55	11.189	1652	1657	1667	rBV	402542	505293	50.57%	6.513%
56	11.451	1697	1700	1703	rBV3	1386	1410	0.14%	0.018%
57	11.493	1703	1707	1708	rBV3	414	485	0.05%	0.006%
58	11.567	1717	1719	1722	rBV4	495	592	0.06%	0.008%
59	11.615	1725	1727	1729	rVB3	987	828	0.08%	0.011%
60	11.756	1745	1750	1755	rBV2	4920	6883	0.69%	0.089%
61	11.902	1772	1774	1776	rBV2	806	680	0.07%	0.009%
62	12.018	1788	1793	1801	rBV	424549	541152	54.16%	6.975%
63	12.085	1801	1804	1812	rVB	7761	11459	1.15%	0.148%
64	12.243	1827	1830	1833	rVB3	1593	1700	0.17%	0.022%
65	12.316	1837	1842	1852	rVV	529753	668404	66.90%	8.616%
66	12.548	1875	1880	1884	rBV6	1689	2847	0.28%	0.037%
67	12.603	1888	1889	1891	rBV	606	447	0.04%	0.006%
68	12.646	1894	1896	1899	rVB3	857	986	0.10%	0.013%
69	12.707	1901	1906	1910	rBV4	1743	2668	0.27%	0.034%
70	12.762	1912	1915	1920	rVB4	2049	3012	0.30%	0.039%
71	12.847	1928	1929	1933	rVB3	887	990	0.10%	0.013%
72	12.902	1933	1938	1944	rBV2	8430	14702	1.47%	0.190%
73	12.963	1946	1948	1953	rVV4	1271	1604	0.16%	0.021%
74	13.011	1953	1956	1959	rVB3	681	1008	0.10%	0.013%
75	13.286	1999	2001	2005	rVB2	1856	1727	0.17%	0.022%
76	13.335	2005	2009	2020	rVB2	34407	45567	4.56%	0.587%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122724\
 Data File : VX044519.D
 Acq On : 27 Dec 2024 14:35
 Operator : JC/MD
 Sample : P5326-06 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 YE685

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\SFAMXLM120524WMA.M
 Title : VOC Analysis

77	13.426	2020	2024	2028	rBV5	2193	3531	0.35%	0.046%
78	13.511	2034	2038	2042	rVB3	6603	9474	0.95%	0.122%
79	13.585	2047	2050	2054	rBV3	784	1158	0.12%	0.015%
80	13.670	2061	2064	2065	rBV2	730	515	0.05%	0.007%
81	13.731	2072	2074	2077	rVB3	635	535	0.05%	0.007%
82	13.780	2077	2082	2088	rBV	8539	13444	1.35%	0.173%
83	13.853	2093	2094	2099	rVB3	658	663	0.07%	0.009%
84	14.054	2125	2127	2130	rBV3	582	666	0.07%	0.009%
85	14.127	2136	2139	2144	rVB2	3398	4499	0.45%	0.058%
86	14.377	2178	2180	2183	rVV4	429	518	0.05%	0.007%
87	14.560	2206	2210	2212	rBV	790	1041	0.10%	0.013%
88	14.694	2230	2232	2234	rBV2	627	467	0.05%	0.006%
89	14.792	2245	2248	2251	rBV3	1275	1736	0.17%	0.022%
90	15.109	2298	2300	2302	rBV2	554	462	0.05%	0.006%
91	15.328	2334	2336	2337	rBV2	1025	673	0.07%	0.009%
92	15.389	2343	2346	2351	rVB3	2041	3171	0.32%	0.041%
93	15.566	2373	2375	2379	rVB4	701	793	0.08%	0.010%
94	15.670	2390	2392	2394	rBV	696	628	0.06%	0.008%
95	15.773	2406	2409	2410	rBV3	592	546	0.05%	0.007%
96	15.816	2414	2416	2418	rBV	557	445	0.04%	0.006%
97	15.913	2430	2432	2435	rBV3	622	749	0.07%	0.010%
98	16.297	2493	2495	2499	rBV4	456	605	0.06%	0.008%
99	16.365	2504	2506	2509	rBV4	692	759	0.08%	0.010%
100	16.682	2557	2558	2561	rVB2	737	457	0.05%	0.006%

Sum of corrected areas: 7757948

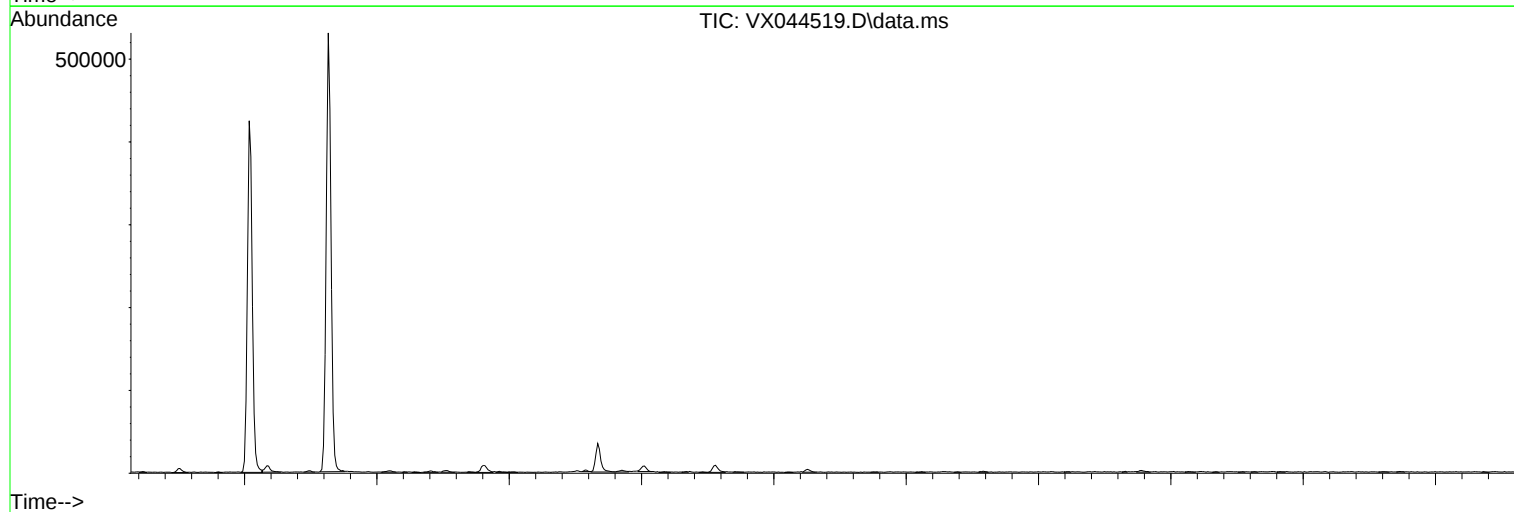
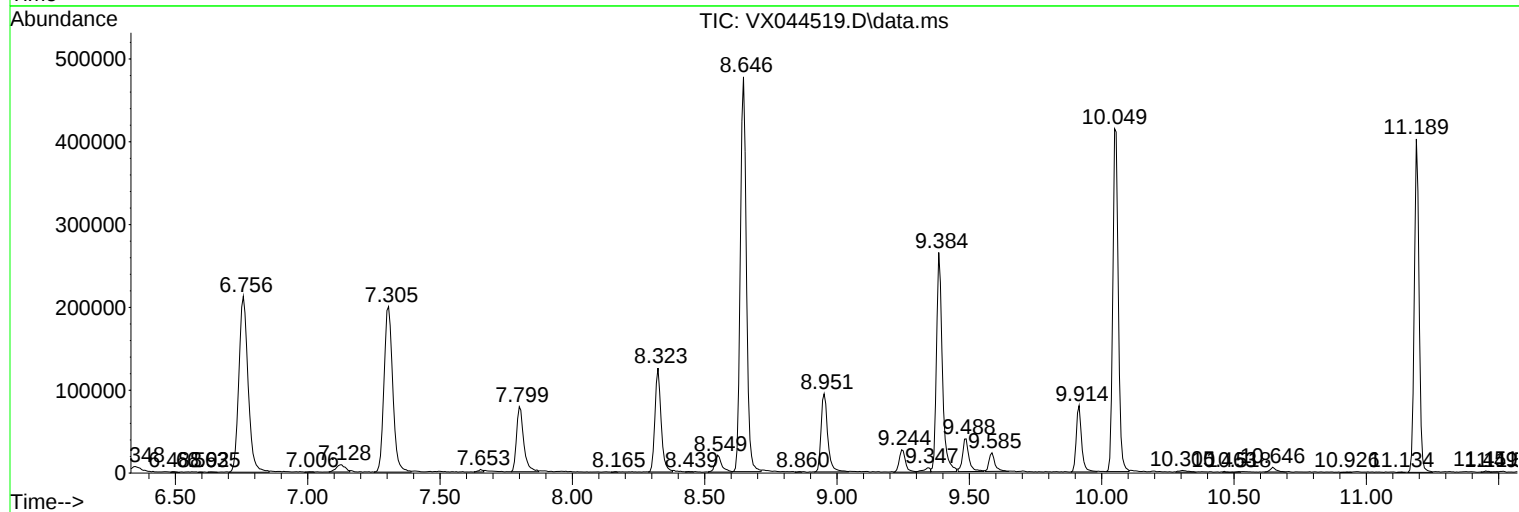
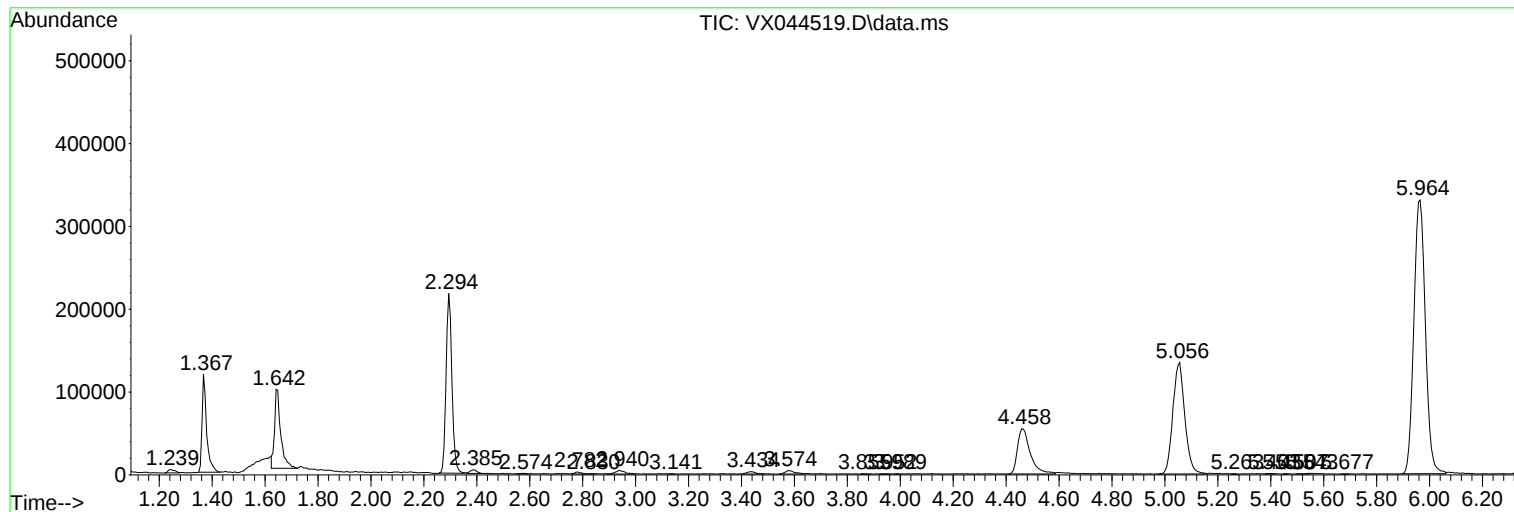
Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122724\
Data File : VX044519.D
Acq On : 27 Dec 2024 14:35
Operator : JC/MD
Sample : P5326-06 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YE685

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122724\
Data File : VX044519.D
Acq On : 27 Dec 2024 14:35
Operator : JC/MD
Sample : P5326-06 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YE685

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

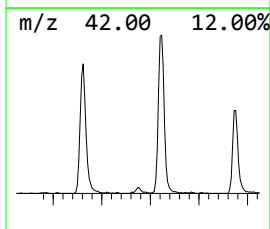
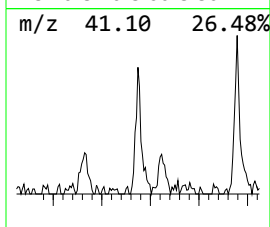
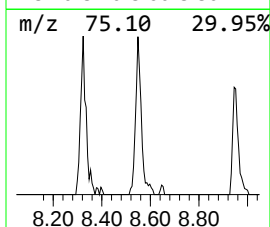
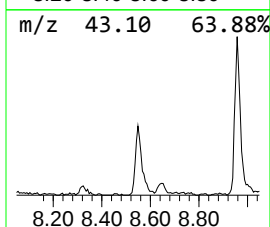
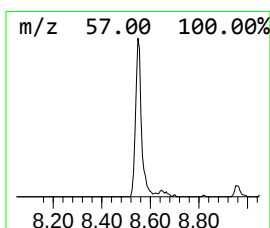
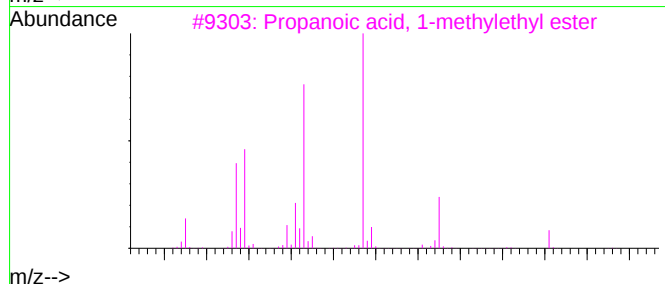
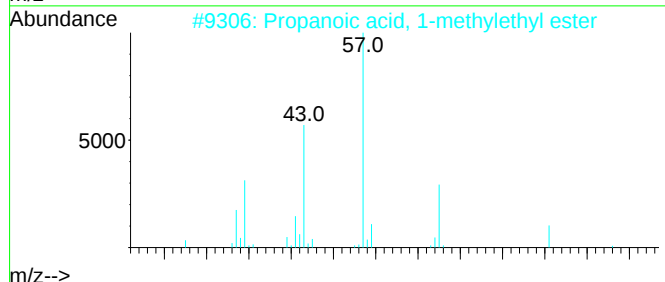
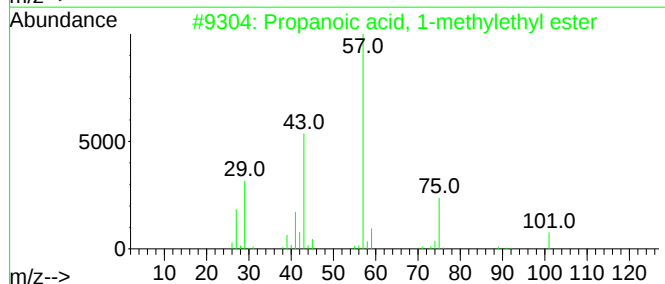
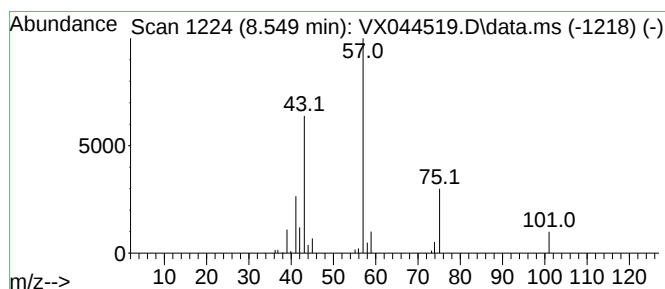
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.549	3.03 ug/L	36042	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	83
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122724\
Data File : VX044519.D
Acq On : 27 Dec 2024 14:35
Operator : JC/MD
Sample : P5326-06 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YE685

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

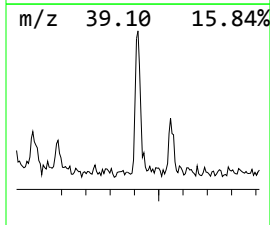
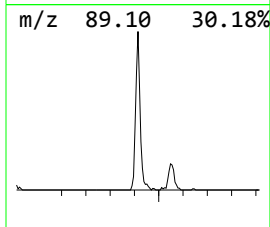
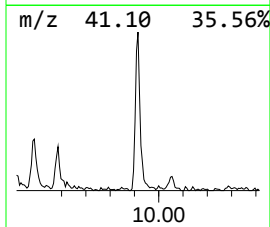
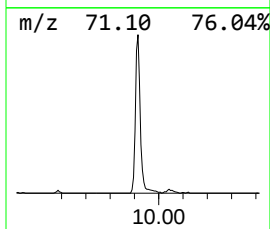
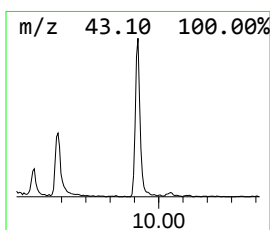
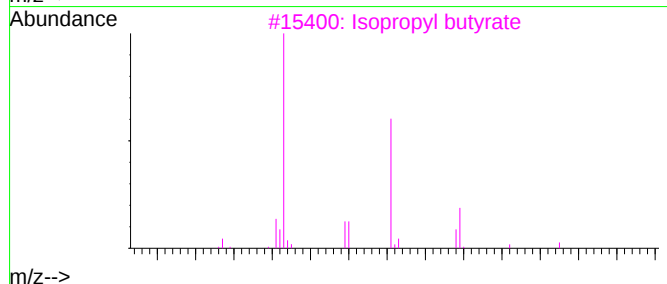
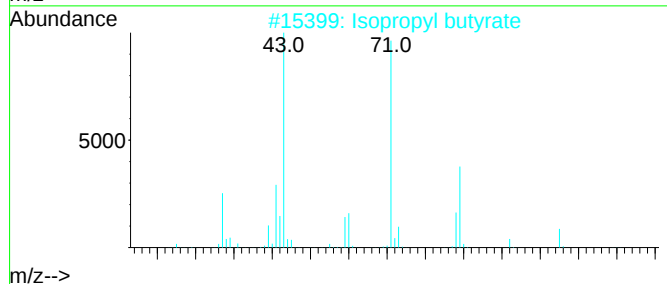
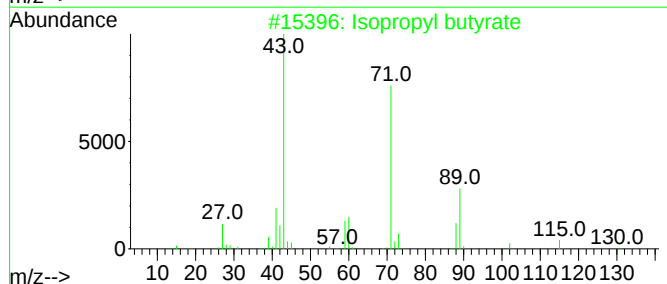
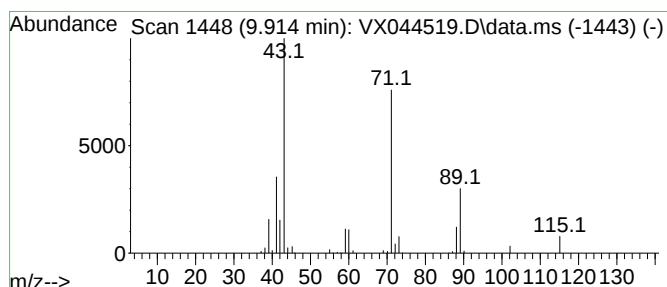
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.914	9.41 ug/L	112000	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	90
2	Isopropyl butyrate	130	C7H14O2	000638-11-9	90
3	Isopropyl butyrate	130	C7H14O2	000638-11-9	78
4	Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	72
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122724\
Data File : VX044519.D
Acq On : 27 Dec 2024 14:35
Operator : JC/MD
Sample : P5326-06 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YE685

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	8.549	3.0	ug/L	36042	2	10.055	594934	50.0
Isopropyl butyrate	9.914	9.4	ug/L	112000	2	10.055	594934	50.0