

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121724\
 Data File : VX044357.D
 Acq On : 17 Dec 2024 17:27
 Operator : JC/MD
 Sample : P5235-16 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AS9

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

Signal : TIC: VX044357.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.245	23	26	27	rBV2	2752	2600	0.26%	0.034%
2	1.367	43	46	54	rBV	108840	121904	12.40%	1.604%
3	1.446	57	59	65	rBV	3534	4677	0.48%	0.062%
4	1.648	88	92	100	rVB	107263	144439	14.69%	1.901%
5	2.294	192	198	209	rBV	177783	285051	28.99%	3.752%
6	2.385	209	213	224	rVB2	8194	15771	1.60%	0.208%
7	2.550	238	240	241	rBV2	1060	626	0.06%	0.008%
8	2.641	254	255	257	rVB2	913	509	0.05%	0.007%
9	2.782	274	278	286	rVB7	1733	3853	0.39%	0.051%
10	2.946	298	305	315	rVB2	10804	26467	2.69%	0.348%
11	3.111	331	332	334	rBV2	742	633	0.06%	0.008%
12	3.184	341	344	346	rBV4	636	645	0.07%	0.008%
13	3.221	348	350	352	rBV	539	433	0.04%	0.006%
14	3.324	363	367	368	rBV2	868	1037	0.11%	0.014%
15	3.428	380	384	385	rBV3	1632	2265	0.23%	0.030%
16	3.586	406	410	418	rVV3	1447	2862	0.29%	0.038%
17	3.861	453	455	457	rBV2	441	424	0.04%	0.006%
18	3.970	471	473	474	rBV	829	433	0.04%	0.006%
19	4.050	485	486	489	rBV3	486	634	0.06%	0.008%
20	4.159	502	504	507	rBV3	481	549	0.06%	0.007%
21	4.391	540	542	545	rBV3	484	604	0.06%	0.008%
22	4.464	546	554	571	rBV	67514	209098	21.27%	2.752%
23	4.732	596	598	600	rBV2	667	549	0.06%	0.007%
24	4.775	603	605	607	rBV3	662	507	0.05%	0.007%
25	4.928	627	630	632	rBV3	444	671	0.07%	0.009%
26	5.056	640	651	668	rVV	131625	410507	41.75%	5.403%
27	5.616	739	743	746	rBV3	611	1081	0.11%	0.014%
28	5.964	788	800	826	rVV2	330024	983258	100.00%	12.941%
29	6.153	829	831	834	rVB3	746	759	0.08%	0.010%
30	6.348	857	863	873	rBV3	7242	20914	2.13%	0.275%
31	6.513	888	890	891	rBV	574	491	0.05%	0.006%
32	6.665	912	915	918	rBV	827	911	0.09%	0.012%
33	6.756	921	930	948	rBV	241070	591218	60.13%	7.781%
34	7.049	975	978	979	rBV3	477	447	0.05%	0.006%
35	7.226	1003	1007	1010	rBV4	733	982	0.10%	0.013%
36	7.305	1012	1020	1035	rVV	203347	448838	45.65%	5.907%

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

37	7.555	1059	1061	1065	rVB3	788	930	0.09%	0.012%
38	7.586	1065	1066	1068	rBV	706	481	0.05%	0.006%
39	7.610	1068	1070	1073	rBV2	801	1195	0.12%	0.016%
40	7.659	1073	1078	1084	rVV	3176	5978	0.61%	0.079%
41	7.799	1095	1101	1116	rBV	83108	158580	16.13%	2.087%
42	8.323	1181	1187	1200	rBV	117436	202132	20.56%	2.660%
43	8.549	1219	1224	1233	rBV	20572	34676	3.53%	0.456%
44	8.646	1234	1240	1251	rBV	449196	706685	71.87%	9.301%
45	8.951	1285	1290	1299	rBV2	94345	153965	15.66%	2.026%
46	9.146	1321	1322	1325	rBV2	653	738	0.08%	0.010%
47	9.244	1334	1338	1347	rBV	29026	42528	4.33%	0.560%
48	9.347	1348	1355	1356	rVV3	4185	6498	0.66%	0.086%
49	9.384	1356	1361	1373	rVV	301107	466646	47.46%	6.142%
50	9.488	1373	1378	1389	rVB	38950	62676	6.37%	0.825%
51	9.585	1390	1394	1401	rVB	17983	26466	2.69%	0.348%
52	9.847	1435	1437	1441	rVB3	628	702	0.07%	0.009%
53	9.884	1441	1443	1444	rBV2	544	425	0.04%	0.006%
54	9.914	1444	1448	1458	rBV	77072	104507	10.63%	1.375%
55	10.006	1461	1463	1465	rBV3	650	516	0.05%	0.007%
56	10.055	1465	1471	1482	rBV	478415	684917	69.66%	9.014%
57	10.646	1564	1568	1578	rBV5	3517	6106	0.62%	0.080%
58	10.731	1580	1582	1584	rVB2	721	481	0.05%	0.006%
59	10.756	1584	1586	1588	rBV	743	691	0.07%	0.009%
60	11.042	1632	1633	1635	rBV	781	690	0.07%	0.009%
61	11.091	1639	1641	1645	rVB3	547	650	0.07%	0.009%
62	11.189	1652	1657	1667	rVV	372394	474914	48.30%	6.250%
63	11.451	1698	1700	1703	rBV3	891	1281	0.13%	0.017%
64	11.573	1718	1720	1723	rVV2	725	692	0.07%	0.009%
65	11.615	1725	1727	1734	rVV3	959	1349	0.14%	0.018%
66	11.756	1746	1750	1760	rBV5	1639	3791	0.39%	0.050%
67	11.865	1766	1768	1772	rBV2	904	1057	0.11%	0.014%
68	11.938	1777	1780	1781	rBV3	950	1085	0.11%	0.014%
69	11.975	1784	1786	1788	rBV	981	671	0.07%	0.009%
70	12.018	1788	1793	1802	rBV	402576	546874	55.62%	7.198%
71	12.195	1819	1822	1823	rBV3	961	990	0.10%	0.013%
72	12.237	1826	1829	1831	rBV3	627	906	0.09%	0.012%
73	12.316	1837	1842	1853	rBV	450039	588395	59.84%	7.744%
74	12.518	1872	1875	1878	rBV3	688	1218	0.12%	0.016%
75	12.694	1901	1904	1905	rBV2	523	445	0.05%	0.006%
76	12.810	1922	1923	1925	rBV2	695	591	0.06%	0.008%

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

77	12.914	1935	1940	1944	rVB5	1119	1794	0.18%	0.024%
78	12.969	1944	1949	1952	rVB4	867	1034	0.11%	0.014%
79	13.121	1973	1974	1977	rVV2	766	560	0.06%	0.007%
80	13.292	1997	2002	2004	rBV4	510	856	0.09%	0.011%
81	13.335	2007	2009	2011	rBV3	474	429	0.04%	0.006%
82	13.511	2036	2038	2042	rVB3	1595	1404	0.14%	0.018%
83	13.682	2064	2066	2069	rBV3	531	493	0.05%	0.006%
84	13.975	2111	2114	2116	rBV2	660	908	0.09%	0.012%
85	14.054	2124	2127	2130	rBV4	623	844	0.09%	0.011%
86	14.444	2189	2191	2192	rBV	603	427	0.04%	0.006%
87	14.499	2199	2200	2203	rBV3	478	448	0.05%	0.006%
88	14.560	2207	2210	2211	rBV	587	612	0.06%	0.008%
89	14.743	2237	2240	2242	rVV2	742	621	0.06%	0.008%
90	14.895	2262	2265	2266	rBV	538	625	0.06%	0.008%
91	15.224	2317	2319	2320	rVB	858	434	0.04%	0.006%
92	15.298	2330	2331	2334	rBV2	574	470	0.05%	0.006%
93	15.523	2366	2368	2370	rVB3	689	549	0.06%	0.007%
94	15.541	2370	2371	2373	rBV2	757	509	0.05%	0.007%
95	15.919	2431	2433	2434	rBV	698	524	0.05%	0.007%
96	15.974	2438	2442	2443	rBV2	837	1130	0.11%	0.015%
97	16.017	2446	2449	2451	rBV3	611	632	0.06%	0.008%
98	16.322	2497	2499	2502	rBV2	573	591	0.06%	0.008%
99	16.352	2502	2504	2507	rVB2	947	741	0.08%	0.010%
100	16.438	2516	2518	2520	rBV3	596	685	0.07%	0.009%

Sum of corrected areas: 7598085

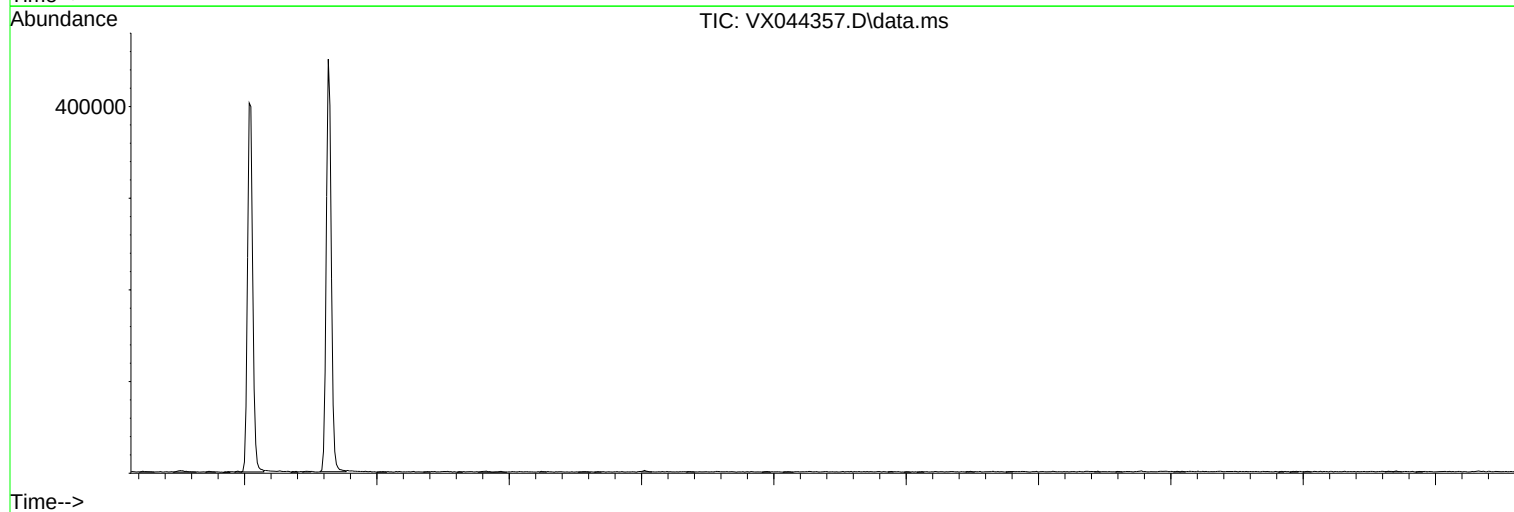
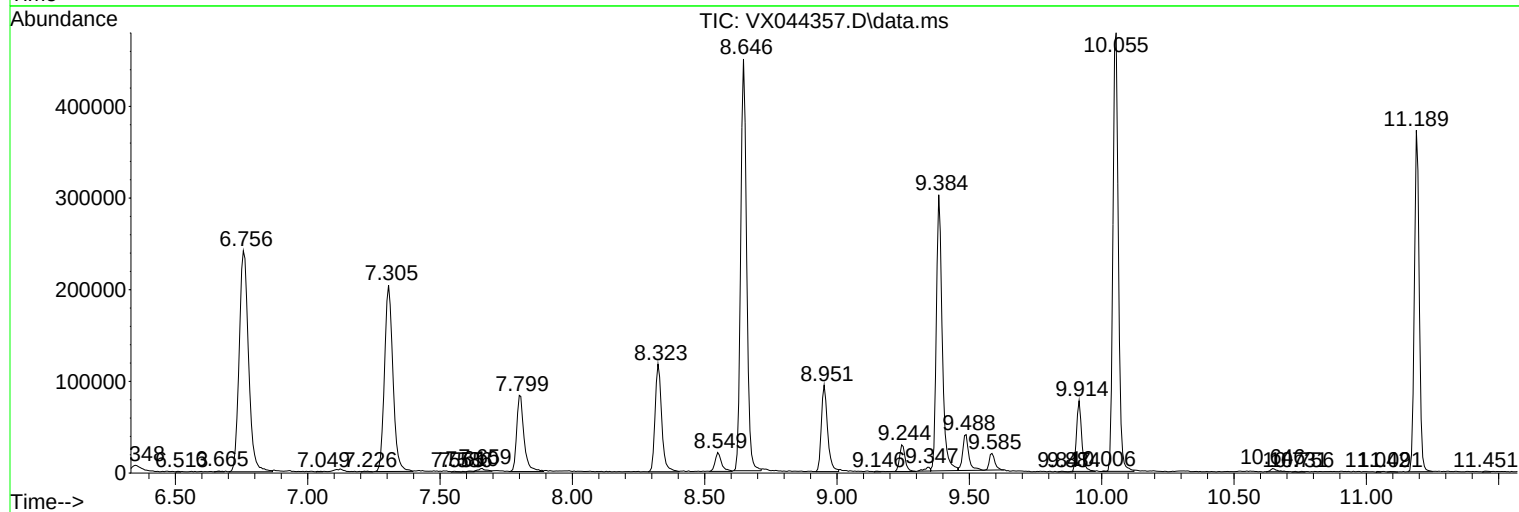
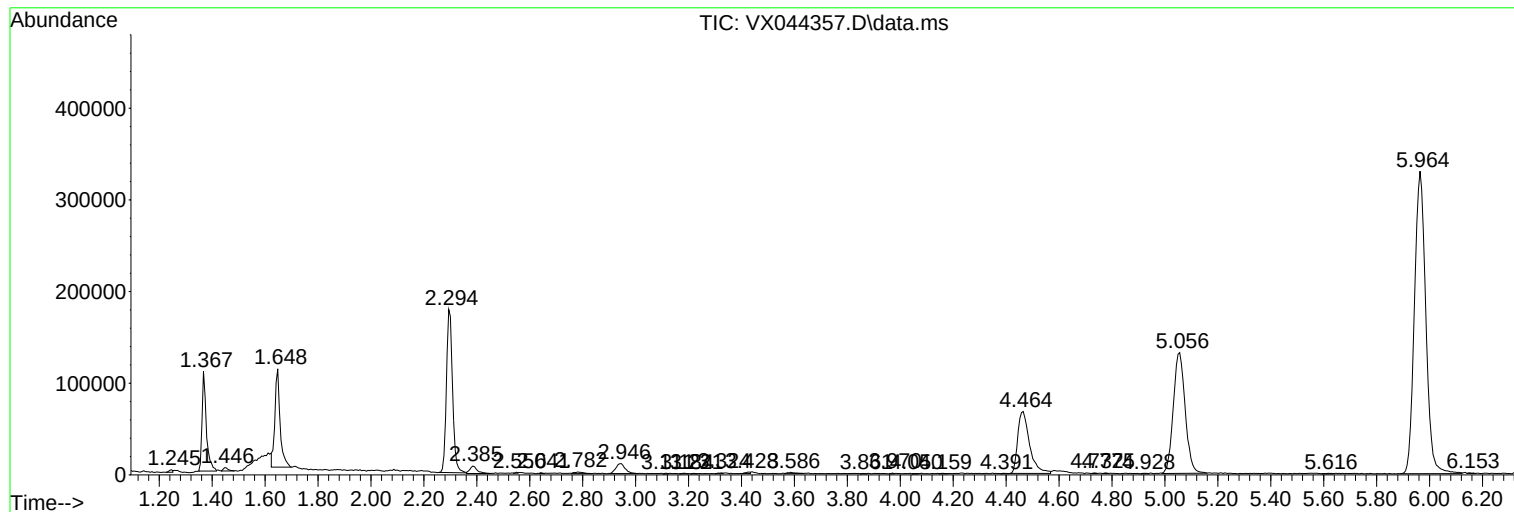
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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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Quant Title : VOC Analysis

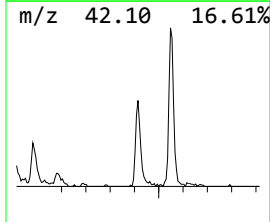
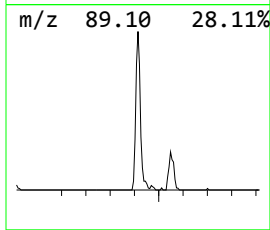
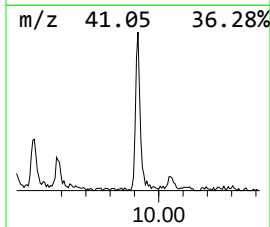
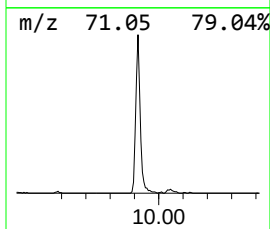
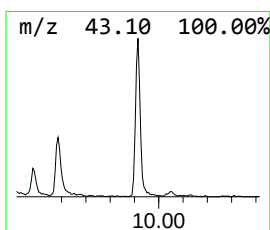
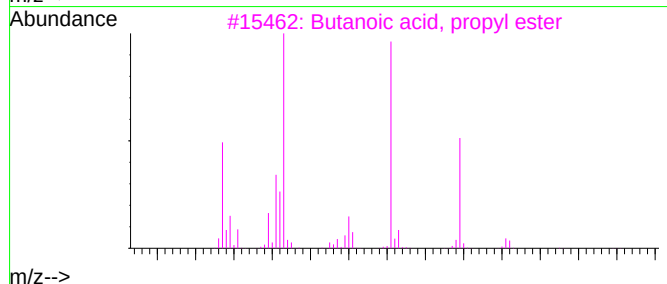
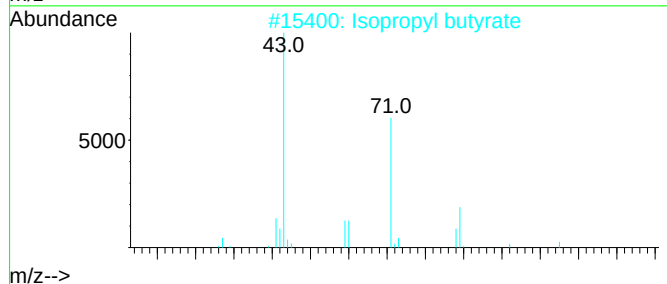
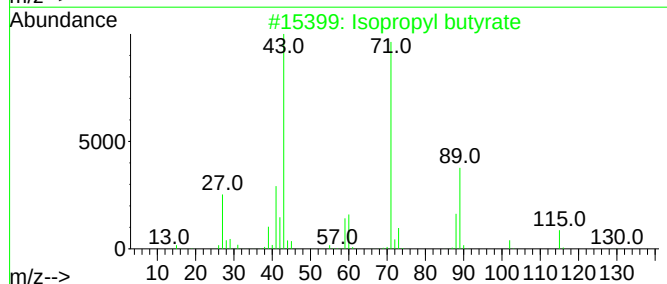
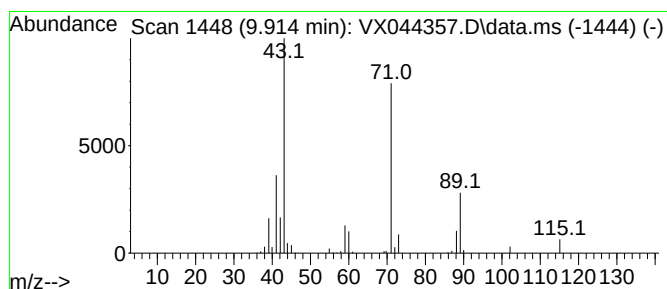
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 6 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.914	7.63 ug/L	104507	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	83
3	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	56



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl butyrate	9.914	7.6	ug/L	104507	2	10.055	684917	50.0