LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121623\
Data File : VX039274.D
Acq On : 16 Dec 2023 08:51
Operator : JC/MD
Sample : 05845-13
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : YCHE9

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: VX039274.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	23	26	32	rBV2	2919	4597	0.33%	0.052%
2	1.368	42	46	55	rVB	116734	134509	9.58%	1.509%
3	1.673	91	96	112	rVB	74435	110726	7.89%	1.242%
4	2.307	194	200	206	rBV	202675	323790	23.07%	3.633%
5	2.374	206	211	223	rVB	361166	575455	41.00%	6.457%
6	2.526	228	236	254	rBV	787203	1403441	100.00%	15.748%
7	2.947	300	305	317	rVB3	4740	11064	0.79%	0.124%
8	3.111	324	332	339	rVV5	3863	9789	0.70%	0.110%
9	3.184	342	344	345	rBV	320	281	0.02%	0.003%
10	3.343	368	370	371	rBV2	261	227	0.02%	0.003%
11	3.605	409	413	414	rBV3	631	809	0.06%	0.009%
12	3.703	428	429	431	rVB	376	201	0.01%	0.002%
13	4.172	504	506	507	rBV	226	206	0.01%	0.002%
14	4.190	507	509	511	rVV	279	214	0.02%	0.002%
15	4.294	525	526	529	rBV2	226	264	0.02%	0.003%
16	4.355	534	536	540	rBV2	183	191	0.01%	0.002%
17	4.446	540	551	562	rBV	77831	223912	15.95%	2.513%
18	4.556	563	569	582	rVB	36249	102032	7.27%	1.145%
19	4.989	630	640	644	rBV	46450	132120	9.41%	1.483%
20	5.385	701	705	707	rBV4	702	1265	0.09%	0.014%
21	5.434	711	713	714	rBV	394	281	0.02%	0.003%
22	5.465	716	718	720	rBV3	952	787	0.06%	0.009%
23	5.678	747	753	760	rBV4	718	1902	0.14%	0.021%
24	5.971	789	801	830	rBV2	305865	938193	66.85%	10.528%
25	6.318	857	858	860	rBV2	253	229	0.02%	0.003%
26	6.403	870	872	873	rBV2	269	201	0.01%	0.002%
27	6.428	873	876	880	rBV2	183	319	0.02%	0.004%
28	6.513	888	890	892	rVV2	258	233	0.02%	0.003%
29	6.562	892	898	900	rVB3	308	488	0.03%	0.005%
30	6.757	919	930	951	rBV	202467	496556	35.38%	5.572%
31	7.129	986	991	997	rBV5	1841	3808	0.27%	0.043%
32	7.306	1012	1020	1038	rBV	188078	420290	29.95%	4.716%
33	7.586	1063	1066	1069	rVB2	175	252	0.02%	0.003%
34	7.830	1100	1106	1109	rBV2	786	1445	0.10%	0.016%
35	7.897	1113	1117	1125	rVV4	1298	2606	0.19%	0.029%
36	8.001	1132	1134	1137	rBV	320	319	0.02%	0.004%

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ClientSampleId :
YCHE9

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

37	8.226	1169	1171	1173	rBV	268	236	0.02%	0.003%
38	8.324	1181	1187	1201	rBV	125339	209688	14.94%	2.353%
39	8.580	1225	1229	1233	rBV2	2558	3787	0.27%	0.042%
40	8.647	1234	1240	1250	rBV	466353	734468	52.33%	8.242%
41	8.854	1272	1274	1277	rVB2	221	193	0.01%	0.002%
42	8.952	1284	1290	1302	rBV	88070	138818	9.89%	1.558%
43	9.159	1320	1324	1329	rVB3	1325	1904	0.14%	0.021%
44	9.275	1339	1343	1350	rVB4	2718	3851	0.27%	0.043%
45	9.330	1350	1352	1355	rBV2	198	261	0.02%	0.003%
46	9.385	1355	1361	1380	rBV	360609	536844	38.25%	6.024%
47	9.610	1395	1398	1404	rVB2	878	1090	0.08%	0.012%
48	9.665	1404	1407	1408	rBV2	336	316	0.02%	0.004%
49	9.756	1419	1422	1423	rBV	191	240	0.02%	0.003%
50	9.799	1426	1429	1431	rBV2	242	258	0.02%	0.003%
51	9.976	1455	1458	1459	rVB2	245	211	0.02%	0.002%
52	10.055	1465	1471	1486	rBV	426053	614997	43.82%	6.901%
53	10.195	1490	1494	1500	rVV	2988	4541	0.32%	0.051%
54	10.305	1506	1512	1518	rBV3	2923	4847	0.35%	0.054%
55	10.653	1563	1569	1577	rVB3	3775	8118	0.58%	0.091%
56	10.805	1591	1594	1597	rVB2	264	289	0.02%	0.003%
57	10.964	1615	1620	1625	rBV	3883	4515	0.32%	0.051%
58	11.024	1626	1630	1634	rVB3	828	1285	0.09%	0.014%
59	11.092	1638	1641	1645	rBV3	1114	1493	0.11%	0.017%
60	11.153	1648	1651	1652	rBV2	791	884	0.06%	0.010%
61	11.189	1652	1657	1664	rVV	341039	440650	31.40%	4.945%
62	11.274	1668	1671	1674	rBV4	948	1020	0.07%	0.011%
63	11.311	1674	1677	1679	rBV2	1185	1424	0.10%	0.016%
64	11.451	1696	1700	1705	rBV	3047	3886	0.28%	0.044%
65	11.585	1719	1722	1724	rBV2	272	283	0.02%	0.003%
66	11.750	1745	1749	1755	rBV	3245	4421	0.32%	0.050%
67	11.878	1767	1770	1772	rBV3	185	211	0.02%	0.002%
68	11.969	1781	1785	1788	rBV2	2485	2873	0.20%	0.032%
69	12.018	1788	1793	1804	rVV	485170	617687	44.01%	6.931%
70	12.225	1823	1827	1834	rVB5	1162	2233	0.16%	0.025%
71	12.317	1837	1842	1850	rBV	499876	640290	45.62%	7.185%
72	12.585	1883	1886	1890	rVB3	435	534	0.04%	0.006%
73	12.616	1890	1891	1894	rBV	205	189	0.01%	0.002%
74	12.683	1899	1902	1907	rBV2	262	435	0.03%	0.005%
75	12.768	1912	1916	1918	rVB3	684	793	0.06%	0.009%
76	12.805	1918	1922	1926	rBV2	299	431	0.03%	0.005%

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ALS Vial : 45 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : YCHE9

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

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Peak separation: 5

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

77	12.939	1941	1944	1952	rBV4	697	1224	0.09%	0.014%
78	13.116	1967	1973	1978	rVB4	1989	2493	0.18%	0.028%
79	13.305	2002	2004	2006	rVB2	306	213	0.02%	0.002%
80	13.372	2011	2015	2018	rBV2	222	316	0.02%	0.004%
81	13.433	2020	2025	2029	rBV3	560	978	0.07%	0.011%
82	13.469	2029	2031	2033	rVB	244	239	0.02%	0.003%
83	13.487	2033	2034	2037	rBV	232	211	0.02%	0.002%
84	13.591	2047	2051	2055	rVB2	2187	2632	0.19%	0.030%
85	13.731	2072	2074	2077	rBV	287	290	0.02%	0.003%
86	13.780	2077	2082	2088	rVB2	2505	3250	0.23%	0.036%
87	13.963	2108	2112	2116	rVV2	1940	2188	0.16%	0.025%
88	14.384	2178	2181	2182	rBV	198	208	0.01%	0.002%
89	14.457	2190	2193	2195	rBV2	321	399	0.03%	0.004%
90	14.554	2207	2209	2213	rBV2	184	239	0.02%	0.003%
91	14.609	2213	2218	2219	rBV3	758	988	0.07%	0.011%
92	14.749	2238	2241	2242	rBV	215	191	0.01%	0.002%
93	14.816	2250	2252	2255	rBV2	249	208	0.01%	0.002%
94	14.987	2276	2280	2281	rBV2	247	327	0.02%	0.004%
95	15.188	2312	2313	2316	rBV2	319	294	0.02%	0.003%
96	15.499	2362	2364	2367	rVB	266	244	0.02%	0.003%
97	15.566	2374	2375	2378	rBV2	309	307	0.02%	0.003%
98	16.280	2490	2492	2493	rBV	291	191	0.01%	0.002%
99	16.341	2500	2502	2503	rBV	252	218	0.02%	0.002%
100	16.658	2552	2554	2559	rVB3	271	261	0.02%	0.003%

Sum of corrected areas: 8911605

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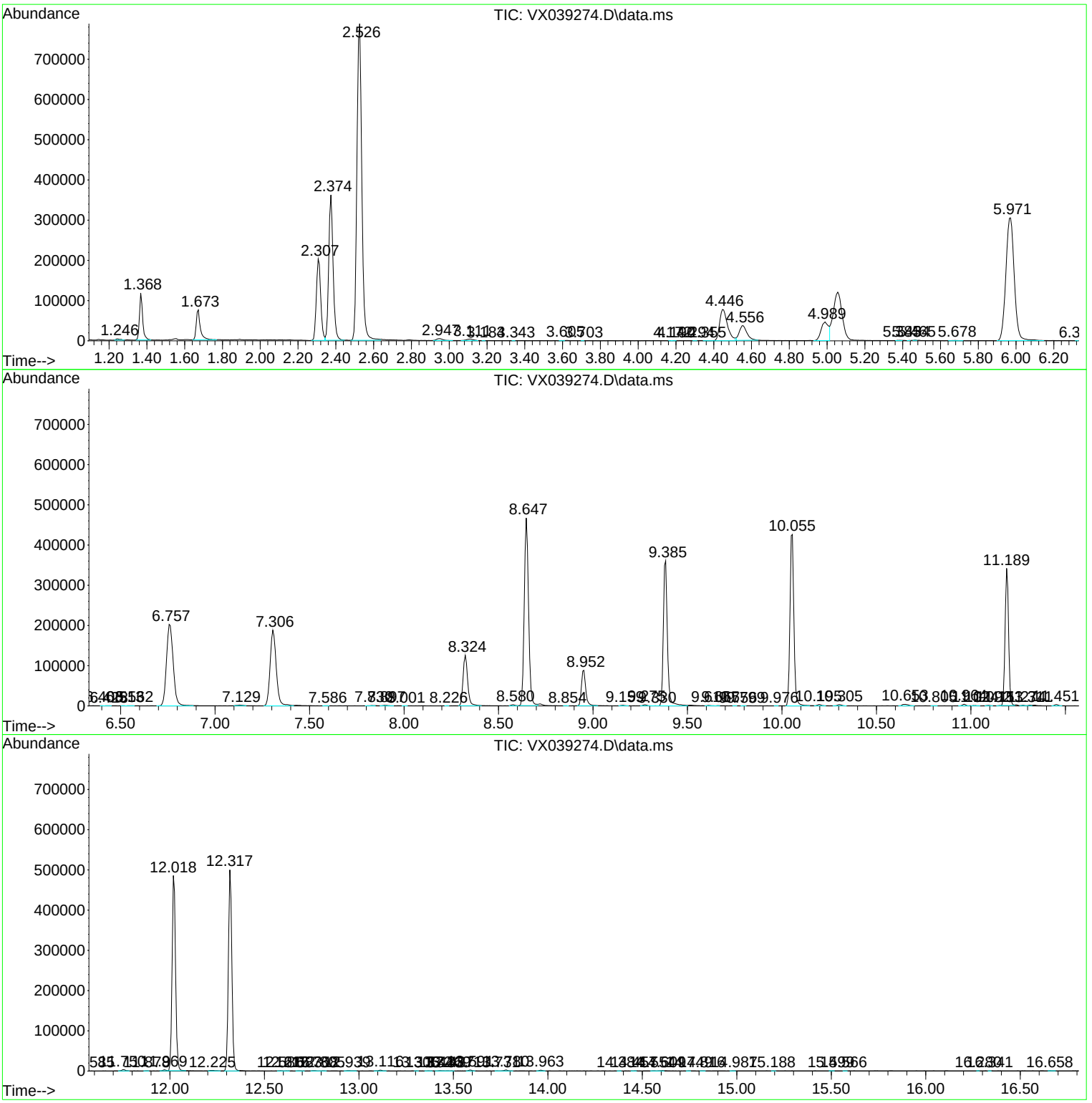
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YCHE9

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



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Quant Title : VOC Analysis

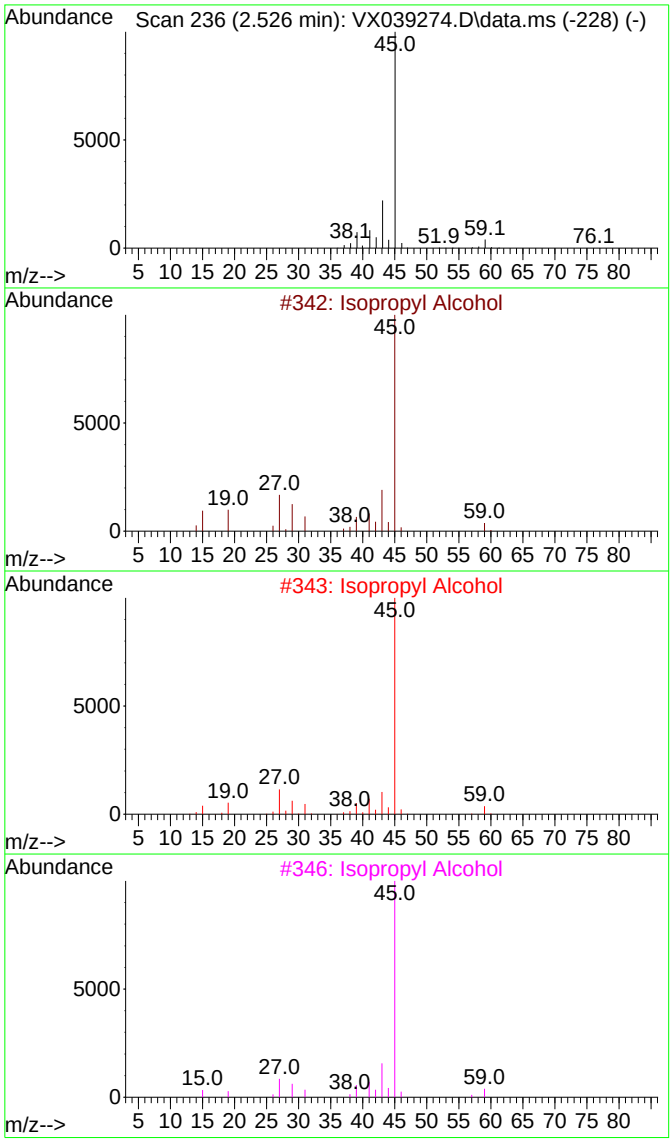
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

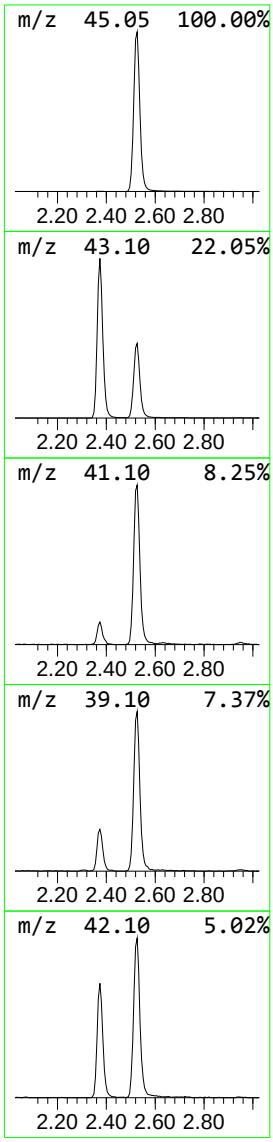
****

Peak Number 1 Isopropyl Alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.526	141.32 ug/L	1403440	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	78
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	64
4	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
5	Hydrazine, ethyl-	60	C2H8N2	000624-80-6	9





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Operator : JC/MD
Sample : 05845-13
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YCHE9

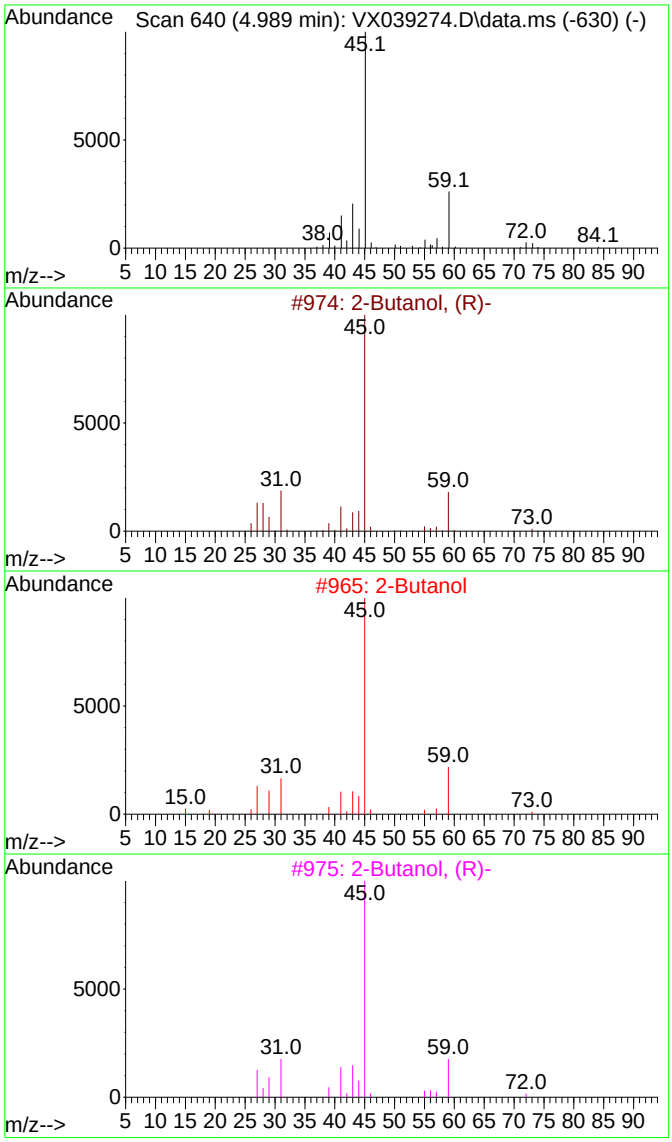
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

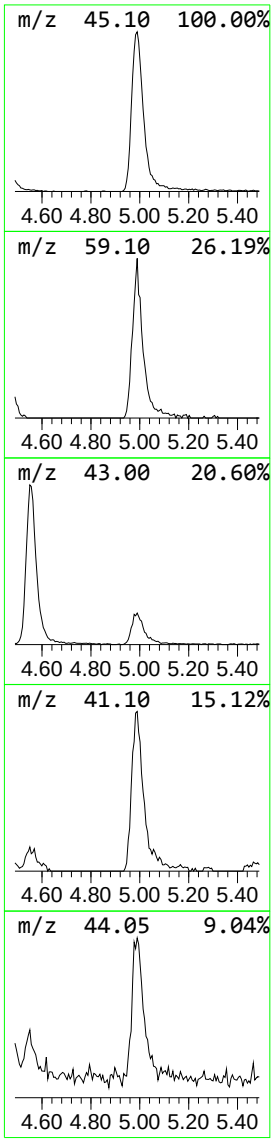
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Butanol, (R)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.989	13.30 ug/L	132120	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, (R)-	74	C4H10O	014898-79-4	83
4	2-Butanol	74	C4H10O	000078-92-2	74
5	2-Butanol	74	C4H10O	000078-92-2	72





Tentatively Identified Compound (LSC) summary

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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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Isopropyl Alcohol	2.526	141.3	ug/L	1403440	1	6.763	496556	50.0
2-Butanol, (R)-	4.989	13.3	ug/L	132120	1	6.763	496556	50.0