

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121623\
 Data File : VX039263.D
 Acq On : 16 Dec 2023 04:40
 Operator : JC/MD
 Sample : 05845-08
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 YCHE4

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\SFAMXML120523WMA.M
 Title : VOC Analysis

Signal : TIC: VX039263.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	27	rBV	2407	2326	0.17%	0.024%
2	1.368	42	46	56	rVB2	119247	146400	10.83%	1.539%
3	1.672	91	96	111	rBV	63239	98575	7.29%	1.036%
4	2.136	168	172	178	rVB3	8477	14196	1.05%	0.149%
5	2.319	194	202	208	rBV2	618623	1104724	81.75%	11.611%
6	2.373	208	211	221	rVB	86238	136363	10.09%	1.433%
7	2.526	229	236	251	rBV	764111	1351370	100.00%	14.204%
8	2.953	298	306	317	rBV2	4930	12540	0.93%	0.132%
9	3.385	374	377	378	rBV2	306	371	0.03%	0.004%
10	3.434	383	385	386	rVV2	273	185	0.01%	0.002%
11	3.526	398	400	401	rBV	251	253	0.02%	0.003%
12	3.611	406	414	422	rVV	13249	31213	2.31%	0.328%
13	3.757	434	438	439	rBV3	746	1066	0.08%	0.011%
14	3.928	462	466	469	rBV2	197	249	0.02%	0.003%
15	4.184	506	508	511	rBV2	236	203	0.02%	0.002%
16	4.452	542	552	563	rBV2	87064	316959	23.45%	3.331%
17	4.989	631	640	643	rBV	32856	84102	6.22%	0.884%
18	5.385	694	705	719	rVB3	22453	66975	4.96%	0.704%
19	5.562	732	734	739	rVV3	297	452	0.03%	0.005%
20	5.708	755	758	760	rVB	317	285	0.02%	0.003%
21	5.781	769	770	773	rBV2	284	234	0.02%	0.002%
22	5.855	780	782	785	rVB2	226	218	0.02%	0.002%
23	5.970	789	801	825	rBV2	294625	912515	67.53%	9.591%
24	6.214	839	841	844	rVB	352	256	0.02%	0.003%
25	6.330	857	860	861	rBV2	288	327	0.02%	0.003%
26	6.470	880	883	888	rBV2	277	463	0.03%	0.005%
27	6.623	906	908	909	rBV2	418	292	0.02%	0.003%
28	6.641	909	911	921	rVB4	1224	2031	0.15%	0.021%
29	6.757	921	930	942	rBV	240615	584796	43.27%	6.147%
30	6.928	956	958	960	rVB2	424	289	0.02%	0.003%
31	7.129	983	991	1002	rBV	30080	67521	5.00%	0.710%
32	7.226	1005	1007	1008	rBV	208	199	0.01%	0.002%
33	7.305	1011	1020	1035	rBV2	187083	414041	30.64%	4.352%
34	7.427	1038	1040	1048	rVB3	2477	4235	0.31%	0.045%
35	7.562	1059	1062	1065	rBV2	278	383	0.03%	0.004%
36	7.775	1094	1097	1099	rBV2	233	299	0.02%	0.003%

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 Title : VOC Analysis

37	7.842	1104	1108	1111	rBV3	475	681	0.05%	0.007%
38	7.903	1113	1118	1126	rVV2	1251	2991	0.22%	0.031%
39	8.324	1181	1187	1198	rVV	128220	207770	15.37%	2.184%
40	8.647	1233	1240	1259	rBV	456091	711840	52.68%	7.482%
41	8.952	1284	1290	1300	rBV	89111	140726	10.41%	1.479%
42	9.275	1338	1343	1347	rVB4	1599	1898	0.14%	0.020%
43	9.384	1355	1361	1377	rBV	369114	553770	40.98%	5.821%
44	9.616	1394	1399	1407	rVV	6940	10909	0.81%	0.115%
45	9.695	1411	1412	1416	rBV2	260	302	0.02%	0.003%
46	9.872	1439	1441	1447	rVB	284	350	0.03%	0.004%
47	9.915	1447	1448	1450	rBV	295	180	0.01%	0.002%
48	9.964	1453	1456	1457	rBV2	197	208	0.02%	0.002%
49	10.055	1465	1471	1485	rBV	503694	719092	53.21%	7.558%
50	10.201	1492	1495	1498	rVB2	348	460	0.03%	0.005%
51	10.256	1503	1504	1507	rBV2	205	177	0.01%	0.002%
52	10.463	1537	1538	1543	rBV	205	229	0.02%	0.002%
53	10.500	1543	1544	1549	rBV2	235	284	0.02%	0.003%
54	10.610	1559	1562	1564	rBV	308	302	0.02%	0.003%
55	10.640	1565	1567	1571	rVV2	487	551	0.04%	0.006%
56	10.701	1575	1577	1583	rVB2	213	391	0.03%	0.004%
57	11.018	1626	1629	1632	rBV4	806	1064	0.08%	0.011%
58	11.091	1637	1641	1644	rVV4	1115	1446	0.11%	0.015%
59	11.189	1652	1657	1665	rVB	363690	456537	33.78%	4.799%
60	11.274	1669	1671	1675	rBV3	496	635	0.05%	0.007%
61	11.311	1675	1677	1679	rBV3	898	1004	0.07%	0.011%
62	11.396	1688	1691	1694	rBV2	163	220	0.02%	0.002%
63	11.616	1725	1727	1729	rBV2	256	263	0.02%	0.003%
64	11.701	1739	1741	1743	rBV	286	205	0.02%	0.002%
65	11.756	1746	1750	1752	rVV3	505	560	0.04%	0.006%
66	11.878	1766	1770	1773	rBV3	214	281	0.02%	0.003%
67	12.018	1788	1793	1802	rBV	540813	698244	51.67%	7.339%
68	12.134	1810	1812	1813	rVB	657	337	0.02%	0.004%
69	12.317	1837	1842	1853	rBV	501043	633660	46.89%	6.660%
70	12.542	1876	1879	1881	rBV2	245	371	0.03%	0.004%
71	12.652	1895	1897	1900	rBV2	232	282	0.02%	0.003%
72	12.750	1911	1913	1914	rBV2	248	251	0.02%	0.003%
73	12.762	1914	1915	1920	rVB2	558	472	0.03%	0.005%
74	12.841	1926	1928	1930	rBV	174	196	0.01%	0.002%
75	12.981	1949	1951	1953	rBV2	181	188	0.01%	0.002%
76	13.048	1958	1962	1964	rBV2	206	296	0.02%	0.003%

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Max Peaks: 100

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Peak separation: 5

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 Title : VOC Analysis

77	13.128	1971	1975	1976	rBV	204	220	0.02%	0.002%
78	13.432	2022	2025	2028	rBV2	474	540	0.04%	0.006%
79	13.591	2048	2051	2053	rVV2	480	419	0.03%	0.004%
80	13.725	2070	2073	2075	rBV2	204	232	0.02%	0.002%
81	13.780	2079	2082	2085	rBV	482	602	0.04%	0.006%
82	13.890	2098	2100	2102	rVB	257	198	0.01%	0.002%
83	13.957	2109	2111	2112	rBV	188	178	0.01%	0.002%
84	14.255	2158	2160	2162	rVB2	265	205	0.02%	0.002%
85	14.316	2168	2170	2176	rVB2	298	474	0.04%	0.005%
86	14.402	2181	2184	2185	rBV2	202	196	0.01%	0.002%
87	14.414	2185	2186	2190	rVB2	338	294	0.02%	0.003%
88	14.457	2190	2193	2199	rBV2	334	429	0.03%	0.005%
89	14.609	2216	2218	2221	rVB2	699	608	0.04%	0.006%
90	14.694	2230	2232	2233	rBV2	224	178	0.01%	0.002%
91	15.438	2352	2354	2355	rVB	370	215	0.02%	0.002%
92	15.456	2355	2357	2358	rBV2	332	333	0.02%	0.004%
93	15.584	2376	2378	2381	rVB2	310	294	0.02%	0.003%
94	15.706	2396	2398	2399	rVB2	350	210	0.02%	0.002%
95	15.975	2439	2442	2445	rBV2	259	305	0.02%	0.003%
96	16.121	2465	2466	2469	rBV3	219	208	0.02%	0.002%
97	16.255	2486	2488	2489	rVB	398	188	0.01%	0.002%
98	16.298	2492	2495	2498	rBV2	316	466	0.03%	0.005%
99	16.511	2527	2530	2532	rBV2	276	394	0.03%	0.004%
100	16.584	2540	2542	2543	rBV2	303	203	0.02%	0.002%

Sum of corrected areas: 9514118

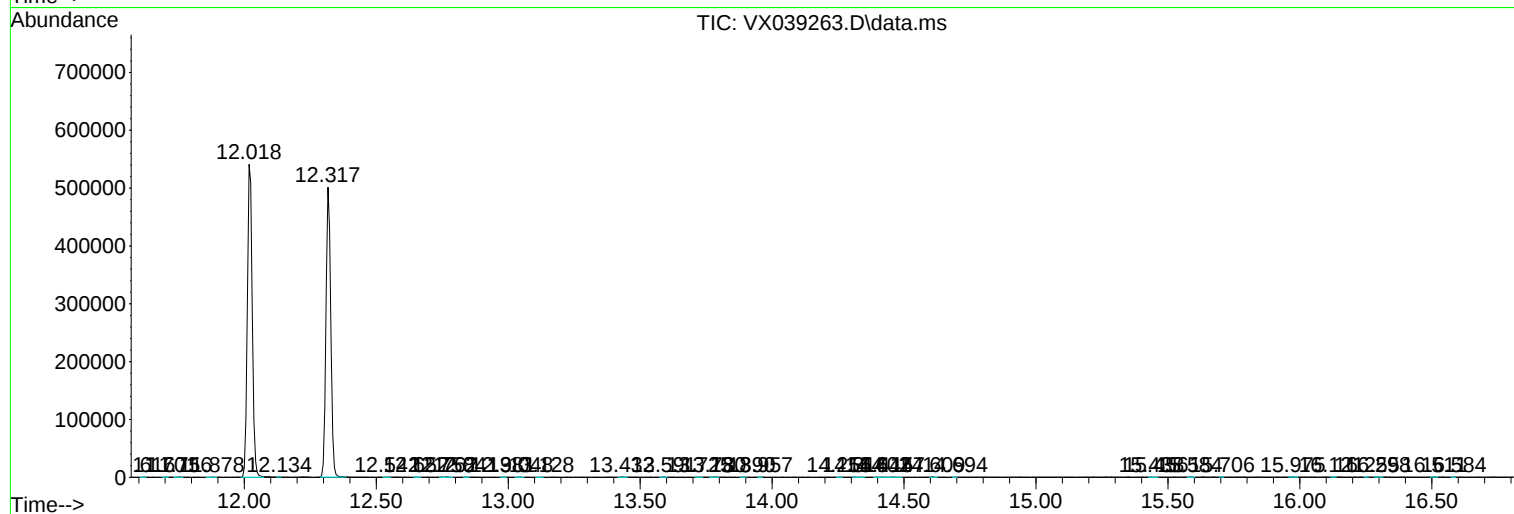
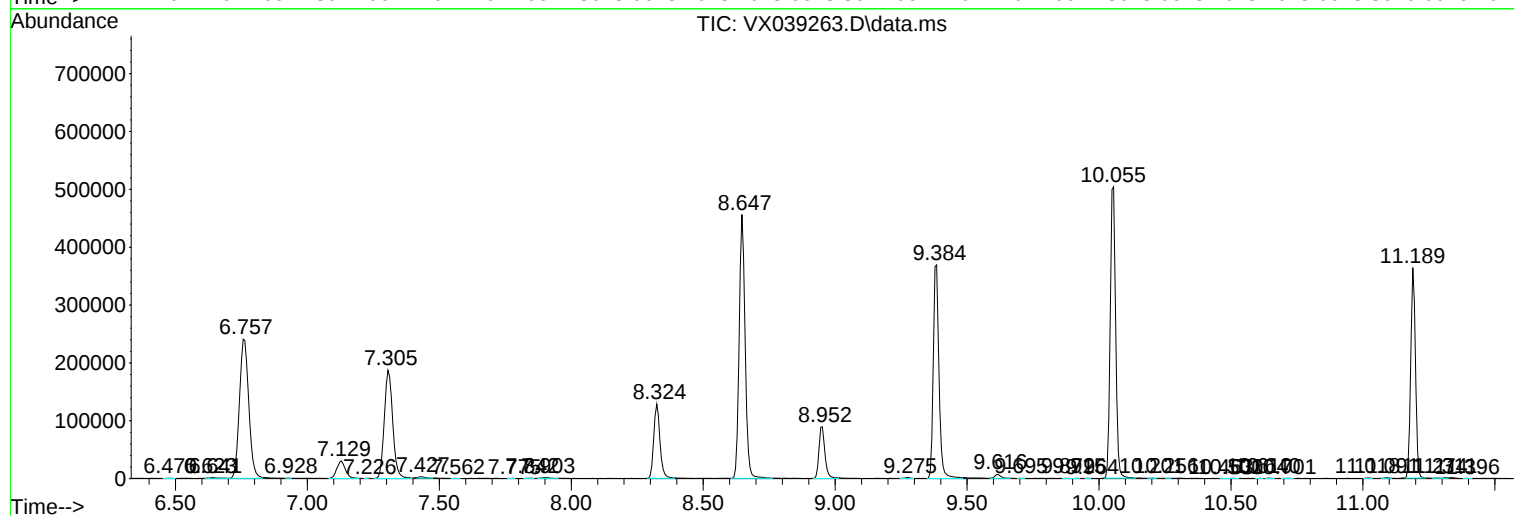
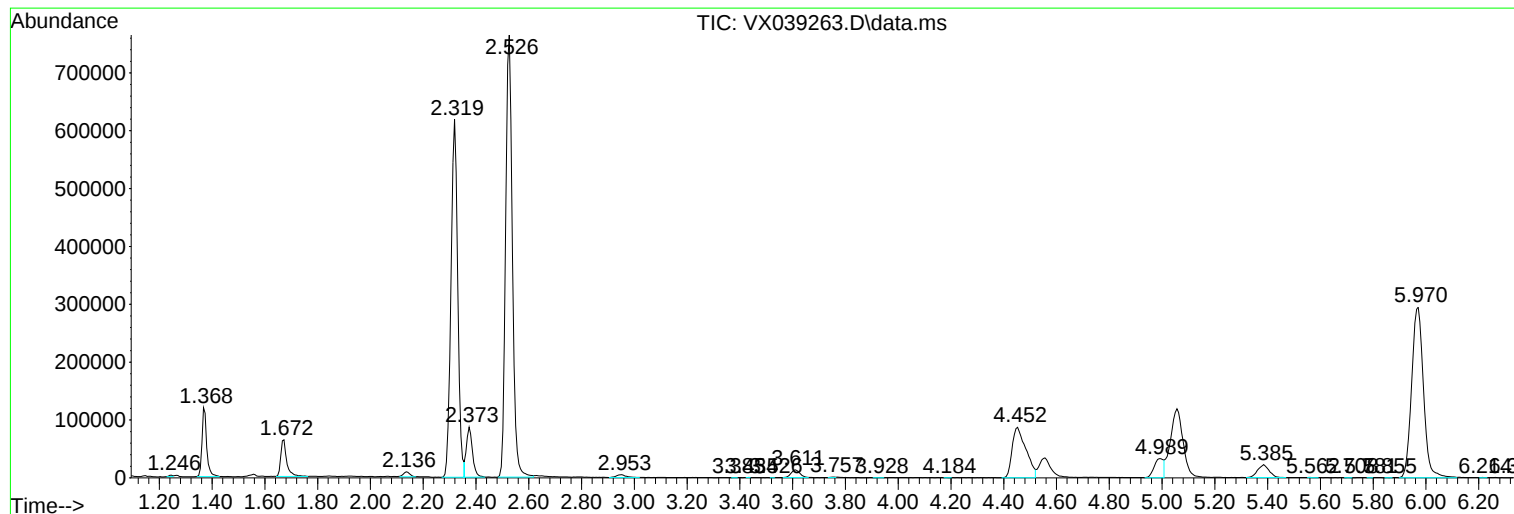
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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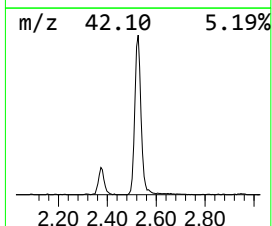
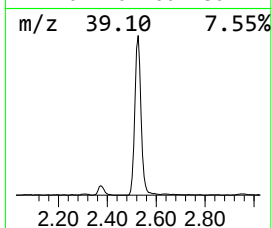
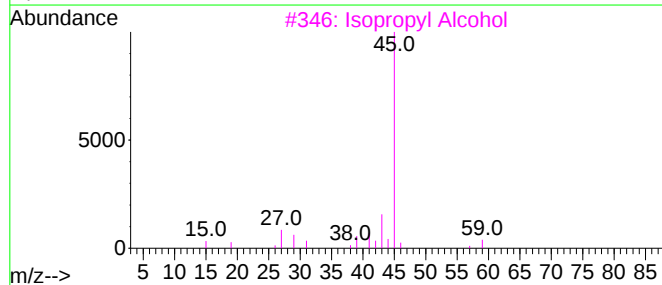
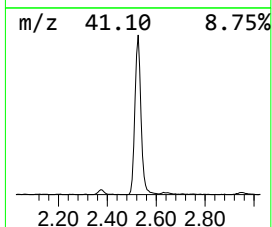
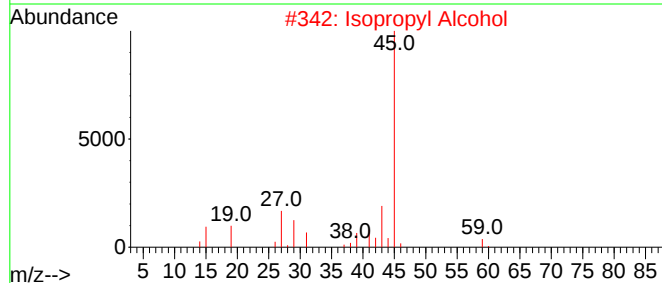
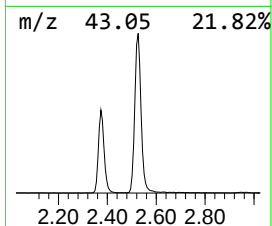
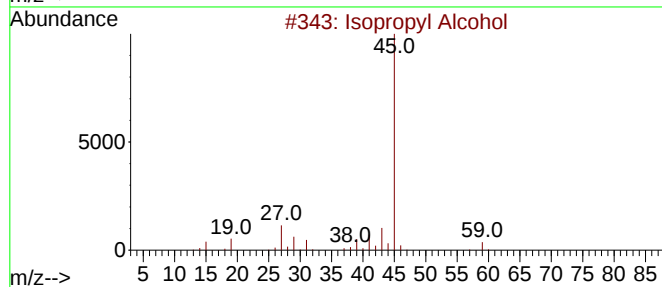
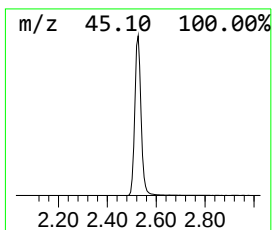
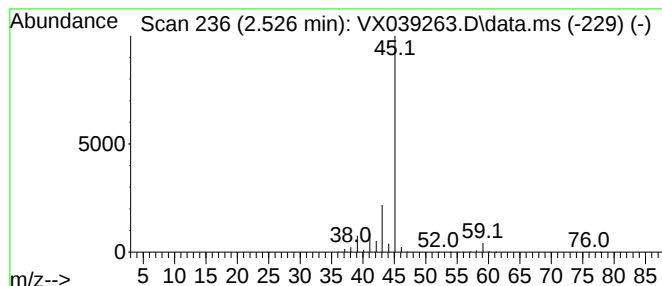
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.526	115.54 ug/L	1351370	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			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9



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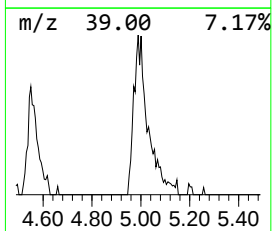
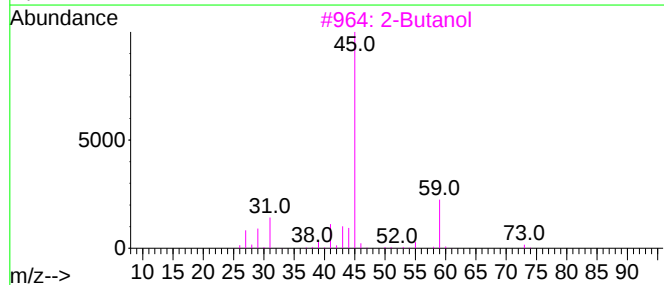
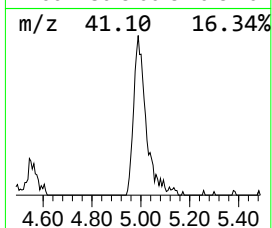
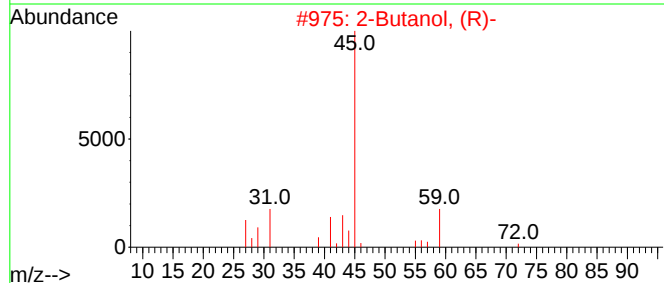
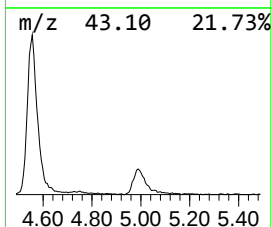
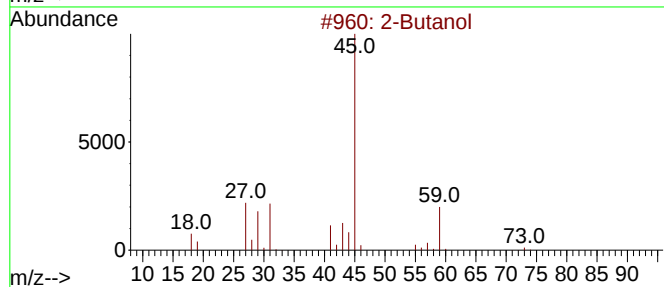
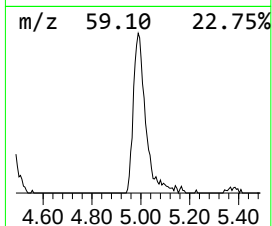
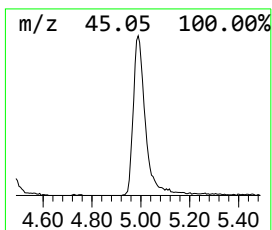
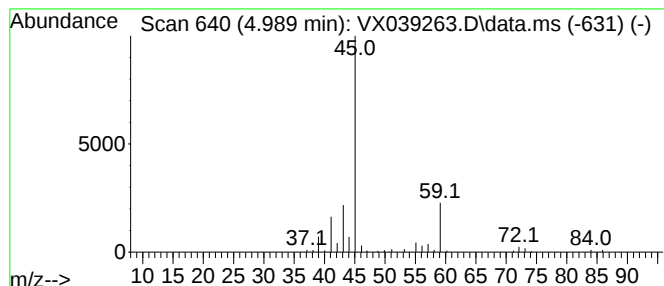
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Butanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.989	7.19 ug/L	84102	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol			74	C4H10O	000078-92-2	78
2	2-Butanol, (R)-			74	C4H10O	014898-79-4	78
3	2-Butanol			74	C4H10O	000078-92-2	72
4	2-Butanol, (R)-			74	C4H10O	014898-79-4	64
5	2-Butanol			74	C4H10O	000078-92-2	64



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl Alcohol	2.526	115.5	ug/L	1351370	1	6.763	584796	50.0
2-Butanol	4.989	7.2	ug/L	84102	1	6.763	584796	50.0