

Returned COMPARE Types in GCxGC-TOFMS Data

Life Science and Chemical Analysis Centre
LECO Corporation, Saint Joseph, Michigan USA

Match:
Benzenepropanoic acid, ethyl ester

Peak True - sample "Beer HA2_1 (splitless)", peak 2 883, at 1350, 2.815 sec, sec

Reference Spectrum - Reference "C2_1 Beer sn50 spcal 10%", Analyte "Benzenepropanoic acid, ethyl ester"

1st Time (s) 1350 1350 1350 1350
2nd Time (s) 2.4 2.8 3.2 3.4

Out of Tolerance:
5-butylidihydro-2(3H)-furanone

Peak True - sample "Beer HA2_1 (splitless)", peak 3 534, at 1584, 2.960 sec, sec

Reference Spectrum - Reference "C2_1 Beer sn50 spcal 10%", Analyte "2(3H)-Furanone, 5-butylidihydro-

1st Time (s) 1584 1584 1584
2nd Time (s) 2.8 3 3.2

Not Found:
Methanesulfonic anhydride/
C2_1 Beer sn50 spcal

Caliper - sample "Beer HA2_1 (splitless)", 276, 0.805 sec, sec to 276, 0.805 sec, sec

Reference Spectrum - Reference "C2_1 Beer sn50 spcal 10%", Analyte "Methanesulfonic anhydride:4"

1st Time (s) 276 276 276 276 276
2nd Time (s) 0.85 0.9 0.95 1 1.05

There are four different "Types" that can be returned in the Type column in the Peak Table of the sample being compared to a Reference. They are, as follows: **Match**, **Out of Tolerance**, **Unknown**, and **Not Found**. A "Match" indicates that the peak in the sample matches all of the criteria (R.T.'s, similarity, concentration, and tolerance) of the peak in the Reference. A return of "Out of Tolerance" means that the peak in the Sample matches all of the criteria of the peak in the Reference, except that its concentration varies from that of the peak in the Reference by more than the set tolerance (in this case, more than $\pm 10\%$ area). A return of "Unknown" means that there is no matching peak in the Reference for that peak in the Sample. A return of "Not Found" means that a peak in the Reference has not been found in the Sample. A return of "Unknown" should not occur for a targeted peak as the "COMPARE" feature is a targeted comparison. In order to return "Unknown" for a peak, that peak must be absent in the Reference and present in the sample. Peaks in the compared Sample that are not included in the Compare Reference will return a type of "Unknown".

For questions on this analysis
e-mail us at: life_science@leco.com

For a complete listing of snapshots and
application notes visit us on the web at
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