Information for FIREX Library "FSL_FIREX2016_v2_2024" generated by NIST as described in paper entitled:

*New library-based methods for non-targeted compound identification by GC-EI-MS*Deborah F. McGlynn, Lindsay D. Yee, H. Martin Garraffo, Lewis Y. Geer, Tytus D. Mak, Yuri A. Mirokhin, Dmitrii V. Tchekhovskoi, Coty N. Jen, Allen H. Goldstein, Anthony J. Kearsley, Stephen E. Stein

Data originated from Library: "FSL_FIREX2016_v2" at *https://nature.berkeley.edu/ahg/resources/* (October 13, 2019).

Software available from: https://chemdata.nist.gov/dokuwiki/doku.php?id=chemdata:nistlibs

Spectrum Annotation:

1) Unidentified spectra have names from the original FIREX collection - beginning with UNK_ followed by sequence number as given in the original library.

2) When names are replaced with names from the NIST library name, the previous name is given as OldName=<Original Name> at the beginning of Comments field

3) Annotation from the original library is the 'Comments' field – this begins with the words: "Fuel Sources"

4) All spectra contain Median_ab= and Total_ab= fields in the Comments field – these are the median and sum of abundances in the spectrum

5) For spectra having significant contamination from Perfluoromethyldecalin (PFMD), major peaks were removed, and a field added to comments in the form:

$$PFMD\_removed=(Freactab=xx\% \ Baseab=yy)$$

where xx is the percent of total initial abundance and yy is the intensity of its base peak (69 m/z) where the base peak intensity in the original spectrum is 999.

6) For spectra where an identification is made with a corrected score over 750 a complex field is added to spectrum *Comments* of the form NIST23(…), where the ellipses (…) represents information described in the an

NIST23(Score=859 MFold=800 ProbNew=79.3 ProbGroup=98.0 nTopGroup=2 MaxScoreDiff=184 DBsCorr=36 ProbCorr=34 RILib=1815 RIFlag=E RevCorr=8)

-Score is the final corrected score
-MFold is the score without corrections (RI-corrected Identity)
-ProbNew is the newly generated 'Probability' for the spectrum – may be followed by ! when very low
-ProbGroup and nTopGroup pertain to a group of highest scoring identifications with a score gap above next rank hits- in this example there are 2 hits that together yield a Probability of 98.0,
-MaxScoreDiff is the largest difference between hits in the hit list
-DBsCorr is the score correction for the Compound Ubiquity Index (CUI)
-ProbCorr is the score correction based on the top two distinct library hits
-RILib is the library Retention Index (standard semipolar)
-RIFlag denotes whether the retention index used is from Experimental (E) or AIRI Calculation (A)
-RevCorr is the correction from averaging initial score with the reverse score to reduce effects due to contaminant peaks