# Application Snapshot

***Instrument: LECO Pegasus BTX***

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*Elemental Analysis | GC Mass Spectrometry | Metallography*

# Non-Target Characterization of Molasses with GC-TOFMS and Deconvolution

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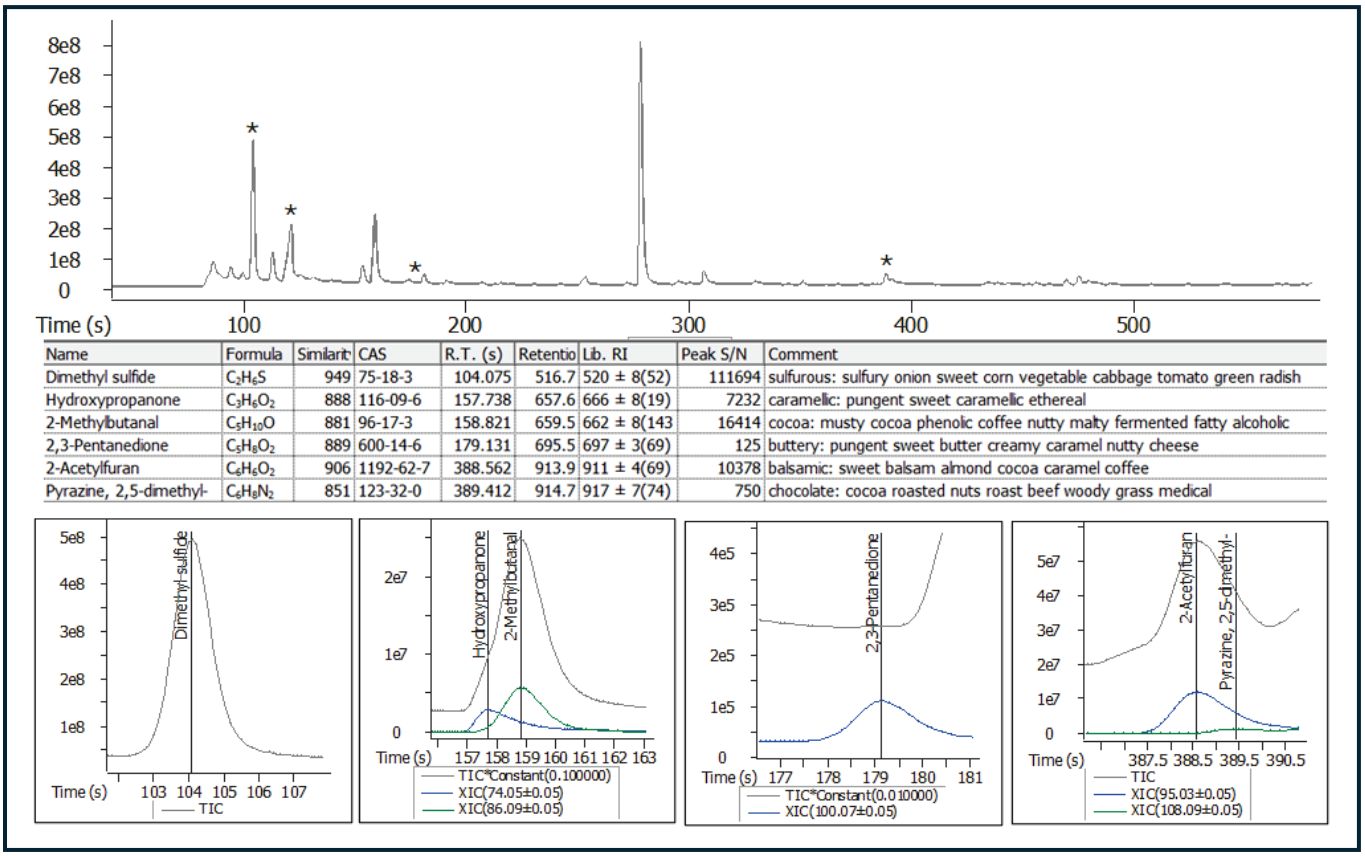
Key Words: Molasses, Food Flavor Fragrance, Deconvolution, Non-Target Analysis, TOFMS, GC, RI




| Name | Formula | Similarit | CAS | R.T. (s) | Retentio | Lib. RI | Peak S/N | Comment |
|---|---|---|---|---|---|---|---|---|
| Dimethyl sulfide | $C_2H_6S$ | 949 | 75-18-3 | 104.075 | 516.7 | 520 ± 8(52) | 111694 | sulfurous: sulfury onion sweet corn vegetable cabbage tomato green radish |
| Hydroxypropanone | $C_3H_6O_2$ | 888 | 116-09-6 | 157.738 | 657.6 | 666 ± 8(19) | 7232 | caramellic: pungent sweet caramellic ethereal |
| 2-Methylbutanal | $C_5H_{10}O$ | 881 | 96-17-3 | 158.821 | 659.5 | 662 ± 8(143 | 16414 | cocoa: musty cocoa phenolic coffee nutty malty fermented fatty alcoholic |
| 2,3-Pentanedione | $C_5H_8O_2$ | 889 | 600-14-6 | 179.131 | 695.5 | 697 ± 3(69) | 125 | buttery: pungent sweet butter creamy caramel nutty cheese |
| 2-Acetylfuran | $C_6H_6O_2$ | 906 | 1192-62-7 | 388.562 | 913.9 | 911 ± 4(69) | 10378 | balsamic: sweet balsam almond cocoa caramel coffee |
| Pyrazine, 2,5-dimethyl- | $C_6H_8N_2$ | 851 | 123-32-0 | 389.412 | 914.7 | 917 ± 7(74) | 750 | chocolate: cocoa roasted nuts roast beef woody grass medical |




***A chromatogram and peak table with representative analytes are shown for the non-target characterization of molasses with the Pegasus BTX. GC-TOFMS and the associated deconvolution algorithms can help you find non-target analytes at high S/N, low S/N, and when coeluting with other features in the sample, as shown with the highlighted examples. These uncovered features have interesting aroma characteristics and likely contribute to the complex aromas of molasses.***

The *Pegasus* BTX is an excellent tool for non-target characterization of complex samples with its enhanced sensitivity, full mass range data, and powerful deconvolution algorithms. You can explore your complex samples beyond the features with the highest S/N to uncover low-level analytes buried in the baseline and untangle coeluting features that would otherwise be obscured. For complex samples, like molasses, these hidden features can have important contributions to the aroma profile and finding them in the data improves the characterization of the sample.