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Quantification of trace O-containing compounds in GTL process samples via Fischer—Tropsch reaction by comprehensive two-dimensional gas chromatography/mass spectrometry

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## **Abstract**

Comprehensive two-dimensional gas chromatography coupled to time-of-flight mass spectrometry (GC×GC-TOFMS) was successfully applied to eight real Brazilian Fischer–Tropsch (FT) product samples for the quantitative analysis of O-containing compounds. It not only allowed identifying and quantifying simultaneously a large number of O-containing compounds but also resolved many co-eluting components, such as carboxylic acids, which co-elute in one-dimensional gas chromatography. The homologous series of alcohols and carboxylic acids as trimethylsilyl derivatives were detected and identified at trace levels. The absolute quantification of each compound was accomplished with reliability using analytical curves. Linear alcohols (from  $C_5$  to  $C_{19}$ ), branched alcohols ( $C_6$ - $C_{13}$ ) and carboxylic acids ( $C_4$  to  $C_{12}$ ) were obtained in the range of 1.58 mg g<sup>-1</sup> to 14.75 mg g<sup>-1</sup>, 0.51 mg g<sup>-1</sup> to 1.12 mg g<sup>-1</sup> and 0.21 mg g<sup>-1</sup> to 1.63 mg g<sup>-1</sup> of FT product samples, respectively. GC×GC-TOFMS provided a linear range (from 0.3 ng  $\mu$ L<sup>-1</sup> to 10 ng  $\mu$ L<sup>-1</sup>), good precision (< 8%), and excellent accuracy (recovery range of 77 % to 118 %) for quantification of individual O-containing compounds in FT product samples. The results can benefit the development of gas-to-liquid technologies from natural gas and guide the choice of an FT conversion process that generates clean products with higher added value.

**Keywords:** Two-dimensional gas chromatography; Gas-to-liquid process; Fischer–Tropsch products; O-containing compounds; Trace analysis

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