

IR Thoughts ~ Thoughts on Information Retrieval, Data Mining, and Search Engines

Building a Hydrocarbons Parser

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POSTED BY EGARCIA IN CHEMICAL MINING, DATA MINING, IR TOOLS, MISCELLANEOUS

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chemical mining, Data Mining, hydrocarbons parser, miner, minerazzi, text mining

Text mining is not limited to computer sciences. It can be applied to chemistry sciences.

Indeed, parsing chemical formulas is not any different from parsing words and phrases, with the added advantage that we can find more practical applications with the former than with the latter.

To illustrate, we are currently building a Hydrocarbons Parser. This is a tool that parses an input chemical formula and predicts the number and types of chemical bonds, normal boiling point temperatures, and few other things. The predicted data can then be compare with experimental results.

Chemical engineers as chemists, chemistry students and their teachers may find this tool useful. This tool is part of an ongoing effort of finding more applications to text mining in other disciplines and fields.

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