

NMRShiftDB RDF #1: Spectra by InChI

Egon Willighagen 

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Keywords

Nmrshiftdb, Sparql

Abstract

Originally, I wanted to include a SPARQL query in my yesterdays blog showing how to retrieve NMRShiftDB spectra based on an InChIKey, but it horribly failed. I have yet to discover why.

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Originally, I wanted to include a SPARQL query in [my yesterdays blog](#) showing how to retrieve [NMRShiftDB](#) spectra based on an InChIKey, but it horribly failed. I have yet to discover why. This morning I discovered that it is specific for that field, and that using the same thing with InChI is no problem: