



SOFTWARE

Mass Spectra of Geochemicals, Petrochemicals and Biomarkers, (SpecData)

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Software
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Description

This high-quality database for the organic, geo-, and/or petrochemist features:

- 1,100 mass spectra of well-defined compounds
- Information including mass spectra, chemical structure, chemical name, molecular formula, molecular weight (nominal mass), base peak, reference, and measurement condition
- Chemical structures elucidated, if necessary, by a variety of techniques including NMR spectroscopy and single-crystal X-ray structure analysis