Mass Spectra of Geochemicals, Petrochemicals and Biomarkers (SpecData) is a high-quality database for organic, geo, and/or petrochemist featuring 1,093 mass spectra of well-defined compounds. Chemical structures elucidated, if necessary, by a variety of techniques including NMR spectroscopy and single-crystal x-ray structure analysis.

The spectra were collected during an extensive project on the occurrence of resistant biomacromolecules and lipids in sedimentary organic matter and mechanisms of fossil fuel generation, as well as the chemistry of organic sulphur in the geosphere. The spectra have been measured by J. W. de Leeuw’s group in the Department of Marine Biogeochemistry at the Netherlands Institute of Sea Research (NIOZ).

The substances have been carefully isolated and purified. Substance classes include saturated and unsaturated aromatic hydrocarbons, aromatic and non-aromatic sulphur and oxygen compounds, terpenes, and steroids and their degradation products.

Specifications
- Mass Spectra: 1,093
- Structures: 1,087
- Unique Compounds: >1,080

Compatibility
Compatible with most current and legacy mass spectrometry data systems. For full compatibility information please visit sciencesolutions.wiley.com/compatibility

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

https://sciencesolutions.wiley.com