

# Mass Spectra of Designer Drugs 2011

**NEW!**

+about 9,700  
ESI MS/MS Spectra

Peter Rösner, Thomas Junge, Folker Westphal, Giselher Fritschi  
Print + CD ROM  
ISBN: 978-3-527-32833-8

## Content

Compounds classified as “designer drugs” have been synthesized since the early 1980s. This is not a precise scientific term and should only be applied to those drugs that are synthesized from common chemicals and skillfully marketed under attractive, often exotic names.

The last decade has seen a proliferation of such substances, such that keeping abreast of this huge number of new drugs is a difficult task for forensic chemists and toxicologists.

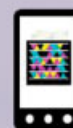
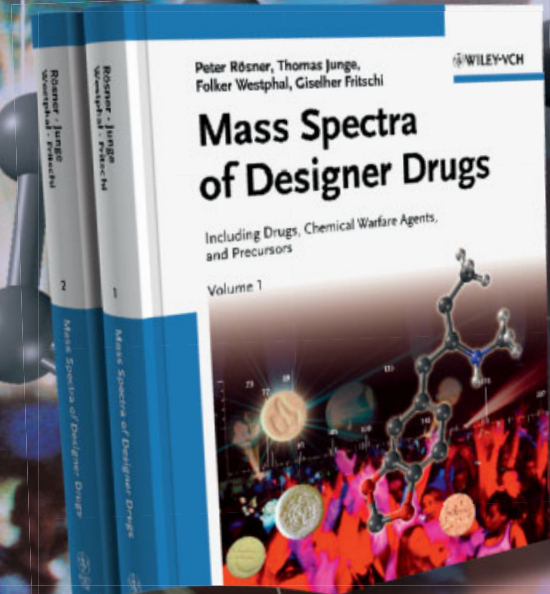
Designer Drugs 2011 covers the entire range of designer drugs up to December 2010. Carefully compiled by the mass spectral experts at the Regional Departments of Criminal Investigation in Kiel and Wiesbaden, Germany, this database includes 11,947 chemical compounds and 14,096 mass spectra **about 1,800 more spectra than the 2010 edition**. In addition, the collection contains pharmaceutical drugs and metabolites – making it the standard in forensic and medical jurisprudence.

LC-MS has become a powerful technique in clinical and forensic toxicology due to its high sensitivity and specificity. In addition to the 14,096 mass spectra of the GC-MS collection 9,653 ESI LC-MS/MS spectra of about 740 compounds have been added to the 2011 edition as a separate database.

The LC-MS data are a valuable and complementary supplement to the GC-MS collection. The spectra have been acquired under standardized conditions and are fully searchable.

## Available Database Formats

- ACD
- Agilent Chemstation
- NIST MSSEARCH
- Finnigan GCQ, SSQ, TSQ, ICIS, ITS40, Magnum
- INCOS
- PE Turbomass
- Shimadzu QP-5000
- Thermo Galactic SpectralID
- Varian Saturn
- VG Labbase, Masslab
- Waters Masslynx
- Xcalibur



Get the free mobil app for your phone  
<http://gettag.mobi>

# Additional Information

Chemical structure, chemical name, molecular formula, molecular weight (nominal mass), biological effect, measurement conditions, average peaks per spectrum: 165, average quality index: 938, and 7,244 experimental Kovats indices.

The data is taken from both legal and underground literature, providing the most comprehensive picture of these compounds worldwide. Edited by Dr. Peter Rösner, Designer Drugs 2011 updates previous editions of the database, and will be updated annually.

## Compound Classes

amphetamines:	904	1-aryl-2-nitroprop-1-enes:	64
methylenedioxyphenethylamines:	514	1-aryl-2-nitrobut-1-ene:	45
phenethylamines:	1032	benzaldehydes:	144
tryptamines:	243	benzodiazepines:	218
piperazines:	356	designer drug isomers:	375
opiates:	146	derivatives:	3258
fentanyls:	240	metabolites incl. derivatives:	2266
cathinones:	98	chemical warfare agents:	67
phencyclidines:	14	designer drug precursors:	588
barbiturates:	56	pharmaceutical drugs incl. metabolites:	3132
arylpropan-2-amines:	102	pesticides:	166
arylbutan-2-amines:	386	explosives:	24
1-aryl-2-nitro-ethenes:	41	controlled compounds:	1043

## Market

Organic chemists involved in structure elucidation; Spectroscopists; Chemical and pharmaceutical companies; Chemistry, biochemistry and pharmaceutical faculties; Governmental institutions; Crime laboratories; Doping control laboratories.



After purchase of the data collection you will receive an instrument manufacturer specific installation key.

**For further information please contact:**

**Dr. Reinhard Neudert**

Phone: +49 (0)6201 606 434

Fax: +49 (0)6201 606 328

Email: [stmdata@wiley-vch.de](mailto:stmdata@wiley-vch.de)

[www.stmdata.de](http://www.stmdata.de)

**Wiley's Online  
World of Analytical Science**

[wileyonlinelibrary.com/subject/analytical-chemistry](http://wileyonlinelibrary.com/subject/analytical-chemistry)

 **WILEY**

 **WILEY-VCH**

