



## **Mass Spectra of Designer Drugs 2012 Upgrade**

Peter Rösner

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Compounds classified as "Designer Drugs" have been synthesized for several decades. 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.

Because of many designer drugs are novel or designed to evade detection, they can be overlooked or difficult to detect or characterize. 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. Compiled by a team originating from the Regional Departments of Criminal Investigation in Kiel, Hamburg, and Wiesbaden, Germany, *Mass Spectra of Designer Drugs* has been developed to help forensics and toxicology labs combat this epidemic.

Mass Spectra of Designer Drugs 2012 covers the entire range of designer drugs up to December 2011. Approximately 70% of the compounds covered in the Designer Drugs do not appear in either NIST 2011 or the Wiley Registry of Mass Spectral Data, 9th Edition.

#### **Specifications:**

#### **Spectra**

Mass Spectra: 16,178
Compounds: 13,420
Structures: 16,178
TSQ-spectra: 9,214
GCQ-spectra: 1,233
CI-spectra: 418
HP-spectra: 1,104
TRACE-spectra: 1,265
GC/MS spectra: 15,991

• Direct insert mass spectra: 179

N. 1 6646 1 5240

• Number of CAS numbers: 5,248 (32.4%)

- Number of measured Kovats Indices: 8,607 (53.2%)
- Number of indication information: 13,131 (81.2%)
- Number of verified MS:2034 (12.5%)
- Number of verified MS by independent measurement:3329 (20.6%)
- Average Peaks/Spectrum: 162.4
- Average Quality Index/Spectrum: 935.7
- Replicate Spectra (same interfacing/ionization mode/system): 240 <=(1.5%)

#### **Compound Coverage**

Compound coverage for individual compounds can be verified at www.compoundsearch.com:

• Amphetamines: 1125

• Methylenedioxyphenethylamines: 590

• Phenethylamines: 1555

Tryptamines: 366Piperazines: 887Opiates: 253

Fentanyles: 326Cathinones: 432Phencyclidines: 17Tropines: 102

Indoles: 244Barbiturates: 75Cannabinoids: 213Cannabimimetics: 165

• Steroids: 140

arylpropan-2-amines: 159
arylbutan-2-amines: 413
indane-2-amines: 46
1-aryl-2-nitro-ethenes: 42

1-aryl-2-nitroprop-1-enes: 651-aryl-2-nitrobut-1-ene: 44

• Benzaldehydes: 146

• Designer drug isomers: 899

• Derivatives: 4533

• Metabolites incl. derivatives: 3298

Chemical warfare agents: 71Designer drug precursors: 725

• Benzodiazepines: 269

• Pharmaceutical drugs incl. metabolites: 4254

Pesticides: 304Explosives: 45

• Controlled compounds: 1550

#### Compatibility

Compatible with most current and legacy mass spectrometry data systems, including:

- ACD/Labs MS Manager
- Agilent Chemstation, MassHunter
- Bruker/Varian
- JEOL
- Leco
- NIST MS Search
- PerkinElmer TurboMass
- Shimadzu GCMS Solution
- ThermoScientific INCOS/GCQ, Spectral ID, XCalibur
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