



Mass Spectra of Designer Drugs 2012

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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
- 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: 366
- Piperazines: 887
- Opiates: 253
- Fentanyles: 326
- Cathinones: 432
- Phencyclidines: 17
- Tropines: 102
- Indoles: 244
- Barbiturates: 75
- Cannabinoids: 213
- Cannabimimetics: 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: 65
- 1-aryl-2-nitrobut-1-ene: 44
- Benzaldehydes: 146
- Designer drug isomers: 899
- Derivatives: 4533
- Metabolites incl. derivatives: 3298
- Chemical warfare agents: 71
- Designer drug precursors: 725
- Benzodiazepines: 269
- Pharmaceutical drugs incl. metabolites: 4254
- Pesticides: 304
- Explosives: 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
- Waters MassLynx

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