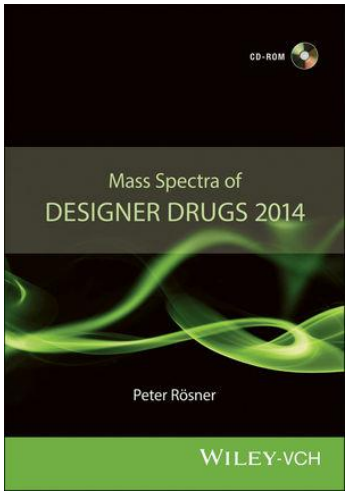
WILEY



Mass Spectra of Designer Drugs 2014

Peter Rösner

ISBN: 978-3-527-33795-8

May 2014

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 2014 covers the entire range of designer drugs up to December 2013. 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: 20,296
Structures: 20,296
TSQ-spectra: 9,361
GCQ-spectra: 1,114
CI-spectra: 508
HP-spectra: 1,361
TRACE-spectra: 1,198
GC/MS spectra: 20,116
Direct insert mass spectra: 180
Different compounds: 16,343
CAS numbers: 6,270 (30.9%)
Measured Kovats Indices: 12,175 (60.0%)
Indication information: 20,296 (100.0%)
Verified MS: 2,212 (10.9%)
Verified MS by independed measurements: 4,523 (22.3%)
Average Peaks/Spectrum: 172.4
Average Quality Index/Spectrum: 942.4/1000
Replicate Spectra (same interfacing/ionization mode/system): 684 <=(3.4%)
Number of compounds by number of mass spectra: 80.5%
Number of mass spectra by number of compounds : 1.2

Compound Coverage

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

Amphetamines: 1,217
Methylenedioxyphenethylamines: 424
Phenethylamines: 1,747
Tryptamines: 323
Piperazines: 813
Opiates: 140
Fentanyles: 281
Cathinones: 576
Phencyclidines: 1
Tropines: 32
Indoles: 850
Barbiturates: 54
Cannabinoids: 34
Cannabimimetics: 523
Steroids: 128
Arylpropan-2-amines: 170
Arylbutan-2-amines: 391
Indane-2-amines: 58
1-aryl-2-nitro-ethenes: 41
1-aryl-2-nitroprop-1-enes: 60
1-aryl-2-nitrobut-1-ene: 44
Benzaldehydes: 126
Designer drug isomers: 1,040
Derivatives: 6,220
Metabolites incl. derivatives: 3,349
Chemical warfare agents: 69
Designer drug precursors: 1,038
Benzodiazepines: 194
Pharmaceutical drugs incl. metabolites: 3,045
Pesticides: 263
Explosives: 26
Controlled compounds: 3,211

Compatibility

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

ACD/Labs MS Manager
Agilent Chemstation, MassHunter
Bruker MSWS
JEOL
Leco ChromaTOF
NIST MS Search
PerkinElmer TurboMass
Shimadzu GCMS Solution
ThermoScientific XCalibur, Chromeleon
Waters MassLynx

Also available in MSP Kofel MassLib format.

Contact: MSP Kofel +41 31 972 31 52 info@msp.ch