Introduction

**Designer Drugs 2017** features 25,114 mass spectra and 19,665 unique compounds predominantly classified as novel psychoactive substances (NPS). The rapid development of these drugs poses serious challenges to current policies, procedures, and methods for detection and identification of these substances. With the dramatic surge of fentanyl addiction, this library helps labs combat the opioid and novel psychoactives epidemics that threaten public health.

Designer Drugs 2017 is the largest collection of chemical signatures of NPS and drugs of abuse in the world. The mass spectra found in this impressive mass spectral reference library were compiled by Dr. Peter Rösner and extensively reviewed by the mass spectral experts Giselher Fritschi and Thomas Junge. The Designer Drugs 2017 mass spectral database was developed to support forensics and toxicology labs to combat this global health epidemic. This edition features the addition of over 1,600 new mass spectra and over 800 new, unique compounds in over 30 different classification groups such as, fentanyl, synthetic cannabinoid, and benzodiazepines. With an average quality index per spectrum of 947.8 and 15,949 Kovats retention indices this spectral library provides comprehensive data on the most up-to-date list of novel psychoactive substances.

Updated annually, the 2017 edition covers the range of known novel psychoactive substances through December 31, 2016. Upgrades are available for purchasers of prior editions. Contact your sales person for upgrade information.

**Key Benefits**

- Mass Spectra: 25,114
- Chemical Structures: 25,114
- Unique Compounds: 19,665
- TSQ spectra: 9,615
- GCQ spectra: 1,075
- CI spectra: 687
- HP spectra: 1,497
- Trace spectra: 1,164
- GC/MS spectra: 24,931
- Direct insert spectra: 183
- CAS RN: 7,604
- Kovats's indices: 15,949
- Indications noted: 25,092
- Externally verified MS values: 2,782
- Independently verified MS values: 7,549
- Average peaks/spectrum: 180.2
- Average Quality Index: 947.8
- Replicate Spectra: 1264

**Instrument Specifications**

Data were acquired on a GCMS TSQ 700, Autosampler CTC PAL A200 SE, split/splitless injector inlet, DB-1 30 m 0.32 mm x 0.25 µm (J&W), Helium in constant linear velocity mode (35cm/s) carrier gas, with an oven temperature of 80°C to 280°C at 15°C/min. Ion source temperature 150°C, interface temperature 280°C, scan range 30-800 u, EI 70 eV.
Author

Peter Rösner, born in Köthen Germany in 1944, studied Chemistry at the University of Kiel where he received a Ph.D in Organic Chemistry in 1981. In the same year he joined the Department of Toxicology at the Landeskriminalamt Kiel where he served as a forensic expert for toxicological analysis until 2004. From 1992 until 2010 he was a lecturer of mass spectroscopy at the University of Kiel. His research activities focused on the structure elucidation of organic compounds by daughter ion mass spectroscopy and the software development for the evaluation and graphical representation of spectroscopic data. He is the developer of the computer program Chemograph and editor of the mass spectral database Designer Drugs.

Compatibility

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

- Agilent Chemstation, MassHunter
- NIST MS Search
- Shimadzu GCMS Solution
- Thermo XCalibur

Compound Coverage

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

- Amphetamines: 2,218
- Methyleneedioxyphenethylamines: 1,225
- Phenethylamines: 2,896
- Tryptamines: 547
- Piperazines: 917
- Opiates: 342
- Fentanyl: 327
- Cathinones: 883
- Phencyclidines: 43
- Tropines: 100
- Indoles: 1,159
- Barbituates: 88
- Cannabinoids: 110
- Cannabimimetics: 901
- Steroids: 191
- Arylpropan-2-amines: 794
- Arylbutan-2-amines: 498
- Indane-2-amines: 95
- 1-aryl-2-nitro-ethenes: 45
- 1-aryl-2-nitrop-1-enes: 70
- 1 aryl-2-nitrobut-1-ene: 45
- Benzaldehydes: 145
- Designer drug isomers: 1,027
- Derivatives: 7,326
- Metabolites (incl. derivatives): 5,610
- Chemical warfare agents: 70
- Designer drug precursors: 1,310
- Benzodiazepines: 297
- Pharmaceutical drugs (incl. metabolites): 5,015
- Pesticides: 328
- Explosives: 54
- Controlled compounds: 5,260

Ordering Information

Mass Spectra of Designer Drugs 2017
CD-Rom ISBN: 9783527343799
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To order:
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