

MS/MS-library Designer Drugs 2009

CI measurements were made with methane as reactand gas
CID measurements were conducted with argon as collision gas

General Data

Number of Mass Spectra: 833
Number of structures: 833
Number of TSQ-spectra: 388
Number of LCQ DECA-spectra: 365
Number of LCQ DECA-spectra ms¹: 108
Number of GC/MS spectra: 468
Number of LC/MS spectra: 365
Number of full Mass Spectra of different compounds: 466
Number of CAS numbers: 319 (38.3%)
Number of indication information: 539 (64.7%)
Average Peaks/Spectrum: 137.2
Number of compounds by number of mass spectra: 55.9%

Compound Structure

Number of amphetamines: 99
Number of methylenedioxyphenethylamines: 66
Number of phenethylamines: 24
Number of tryptamines: 13
Number of piperazines: 36
Number of opiates: 19
Number of cathinones: 13
Number of phencyclidines: 5
Number of barbiturates: 4
Number of arylpropan-2-amines: 19
Number of arylbutan-2-amines: 57
Number of benzylamines: 1
Number of benzaldehydes: 8
Number of designer drug isomers: 15
Number of derivatives: 15
Number of metabolites incl. derivatives: 129
Number of chemical warfare agents: 5
Number of designer drug precursors: 13
Number of benzodiazepines: 5
Number of pharmaceutical drugs incl. metabolites: 252
Number of pesticides: 34
Number of explosives: 7
Number of controlled compounds: 36