Spectra submission

Spectrum Format

2 columns separated by a whitespace, e.g.

190.0000 82.61

190.5000 87.23

191.0000 97.93

191.5000 106.35

192.0000 112.84

192.5000 118.06

193.0000 122.06

193.5000 124.98

194.0000 127.03

194.5000 128.31

195.0000 129.16

195.5000 129.73

Store as text file with .xy extension

Textfile with additional information

Filename, compound name, smiles, solvent, instrument