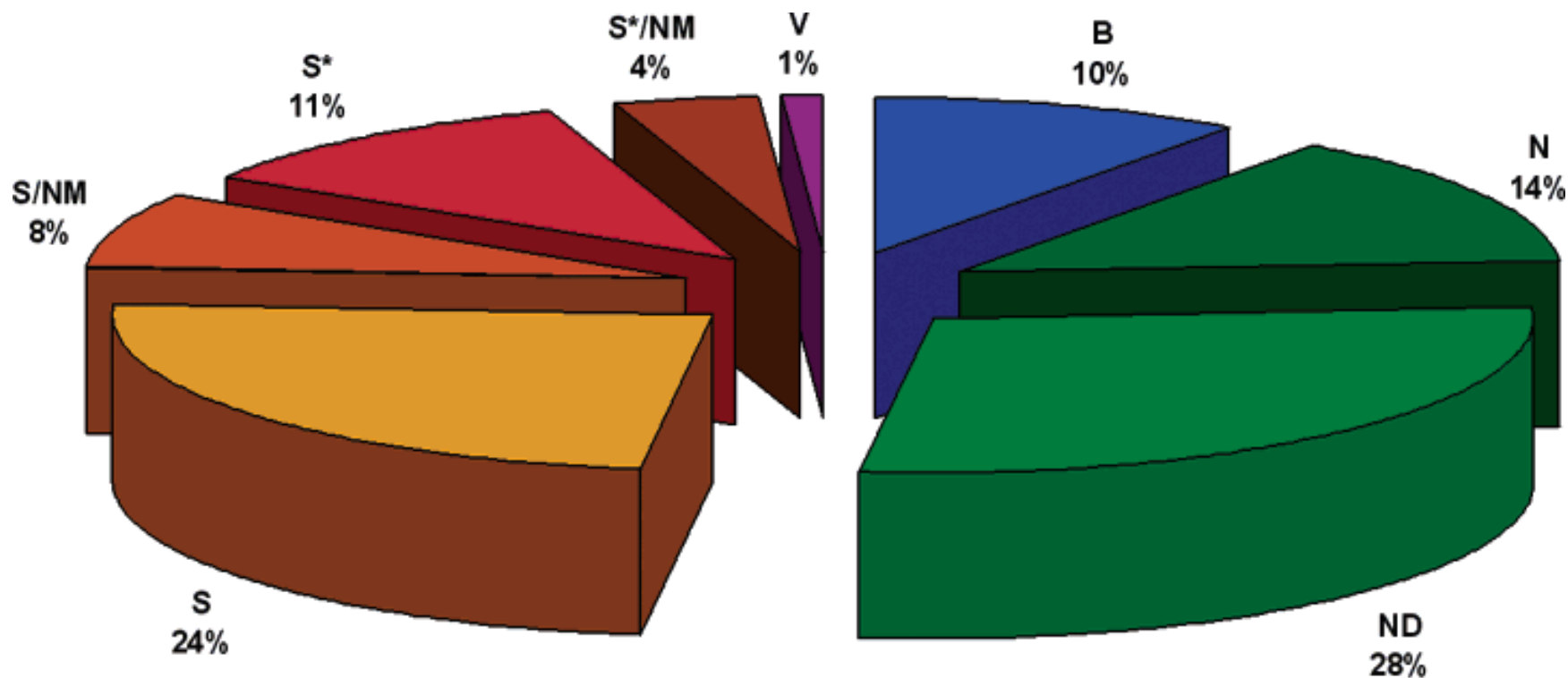


Hands-on approach to early-stage drug discovery

Experimental course of 10 ECTS point

University of Southern Denmark (SDU), Department
of Physics, Chemistry and Pharmacy

Anticancer drugs (N = 175) developed in the period 1940–2006



N = natural product, **ND** = modification of natural product (semi-synthesis), **B** = peptides and proteins, **S*** = total synthesis of a natural products (often simple natural products), **S** = synthetic substances found by random screening for biological activity.

Hands-on approach for identifying bioactive natural products from complex extracts using bioassay-guided fractionation



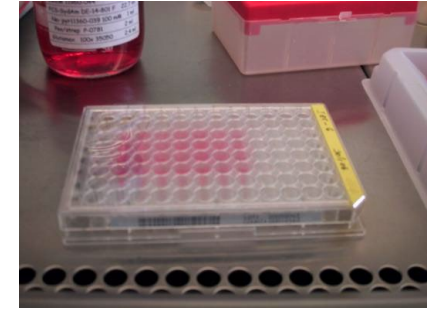
Extraction of biological material

Terrestrial and aquatic plants, marine organisms or micro-organisms.



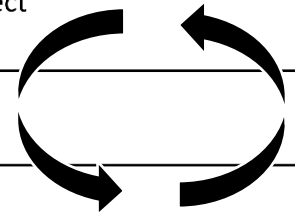
Crude extract

Evaporation of solvent and preparation for testing and fractionation.



Testing in relevant *in vitro* bioassays (bioactivity evaluation)

(i) Anti-inflammatory activity
(ii) Antiproliferative activity/cytotoxicity
(iii) Antibiotic effect
Etc.

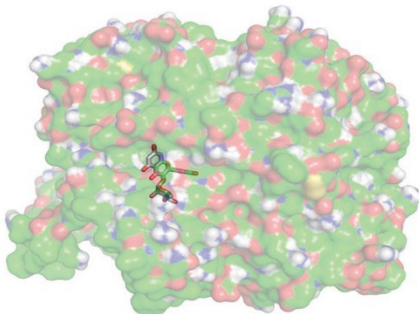


Fractions

Fractionation of crude extract and active fractions by flash column chromatography and prep. HPLC. Typically multiple rounds of fractionation of active fractions.

In silico

Molecular modelling of BNPs in target proteins (computational chemistry). Elucidation of possible mechanisms of action.



Single bioactive natural products (BNPs)

Identification of BNPs using spectroscopic techniques such as UV, LC-MS and NMR.

