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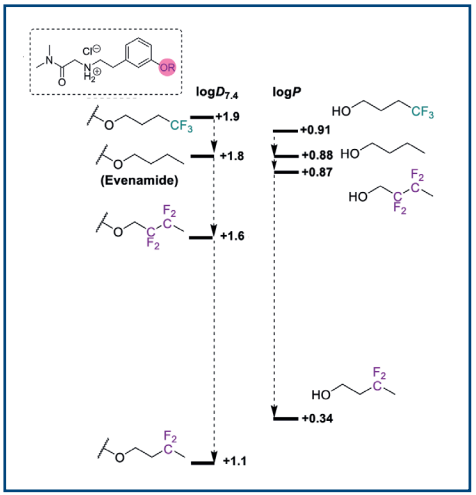
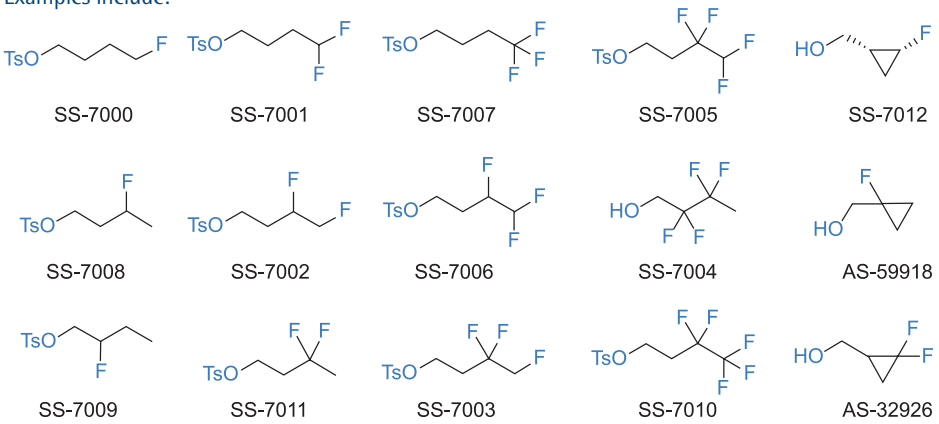
Fluorinated hydrophobic groups for lipophilicity tuning in drug development

UNIVERSITY OF Southampton

Optimization of compound lipophilicity is a key aspect of drug discovery, collaborating with Professor Bruno Linclau and Mariana Manso at the University of Southampton, Key Organics are delighted to be able to offer toolkit compounds to enable researchers to manipulate physical properties.



Examples include:



Reference: Systematic Investigation of Lipophilicity Modulation by Aliphatic Fluorination Motifs; Linclau et al; *J Med Chem 2020, 63, 3, 1002–1031*

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Functional Group and Substructure Group Classes

BIONET Functional Groups

- Alcohols
- Aldehydes
- Amines
- Amino Acids
- Aromatic OH
- Boron Compounds
- Carboxylic Acids
- Diamines
- Dicarbonyls 1,3
- Esters
- Fluorinated Compounds
- Hydrazides
- Hydrazines
- Hydroxylamines
- Ketones
- Miscellaneous Functional Groups
- Nitriles
- Protected Compounds
- Reactive Halides
- Saturated Compounds
- Spiro Compounds
- Sulphonyl Chlorides
- Thiols

BIONET Substructure Groups

- Anilines
- Azaindoles
- Benzimidazoles
- Benzodioxepines
- Benzodioxines
- Benzodioxoles
- Benzofurans
- Benzothiadiazole
- Benzothiazines
- Benzothiazoles
- Benzothiaphenes
- Benzoxazines
- Benzoxazoles/Benzisoxazoles
- Furans
- Imidazoles
- Indoles
- Isoindoles
- Isoquiolines
- Isothiazoles
- Isoxazoles
- Naphthalenes
- Naphthyridines
- Other Ring Systems
- Oxadiazoles
- Oxazoles
- Piperidines
- Pyrans
- Pyrazoles
- Pyrazolopyridines
- Pyridines
- Pyrimidines
- Pyrroles
- Pyrrolidines
- Quinazoline
- Quinolines
- Quinoxalines
- Thiadiazoles
- Thiazolanes
- Thiazoles
- Thiaphenes
- Triazoles

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