### Southampton Commercialisation of small fluorinated hydrophobic Key Organics groups for lipophilicity tuning in drug development Chemistry Innovation Quality

### Mariana Manso,<sup>1</sup> Bruno Linclau<sup>\*,1</sup> and Steve Brough<sup>\*2</sup>

<sup>1</sup>Chemistry, University of Southampton, Highfield, Southampton, SO17 1BJ, UK; <sup>2</sup>Key Organics, Camelford, Cornwall PL32 9RA, UK E-mail: m.g.manso@soton.ac.uk; bruno.linclau@soton.ac.uk; steveb@keyorganics.net.

# Lipophilicity is an important parameter in drug discovery

• Next to bioactivity, optimisation of lipophilicity is crucial in drug development.

## Fluorination as a tool to finetune lipophilicity<sup>1-3</sup>

extensive study of the An effects of aliphatic fluorination on lipophilicity can be found on Investigation of Lipophilicity



#### **Incorporation of the fluorinated moiety:** 4M HCl in ROTs or ROTf Dioxane HCI OH N Boc $Cs_2CO_3$ (89 %- quant) Boc O DMF (43-75 %) Typical introduction with a tosylate or triflate functional group. Introduction via the alcohol is in development. Stock of compounds available $\log D_{7.4}$ log*P* HO CF<sub>3</sub> **.9 (**∆ **+0.1)** Ts O´ HO Ts O<sup>´</sup> **TsO** •+0.91 (<u>∧</u> +0.03) **-+0.88** HO +1.8 SS-7012 **SS-7000 SS-7001 SS-7007 SS-7005 -** +0.87 (∆ -0.01) $F_2$ (Evenamide) HO HO Ts O Ts O ΗÓ +1.6 (**∆** -0.2) AS-59918 **SS-7008 SS-7002 SS-7006 SS-7004** Ts O HO

AS-32926



**SS-7003** 

#### **Acknowledgements:**

**SS-7009** 

SS-7011

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#### **References:**

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