Public knowledge of the compd found on the website (left mouse click).

Link_to_PubChem for compound 212581

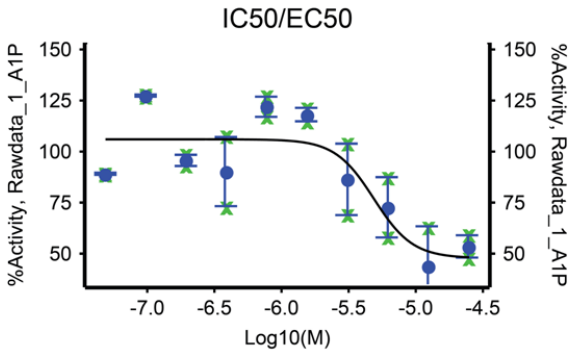
Position of the compd in the 384-screening plate.

Position on plate: G16

RelActDiff: Difference of percent activity between the left and the right asymptot of the IC50 values.
HillCoefficient: It is used to estimate the number of ligands that are required to bind to the target (ideally = 1 slope of the curve at the point of IC50).
ChiSquared: the squared deviation from the fitted line.

IC50

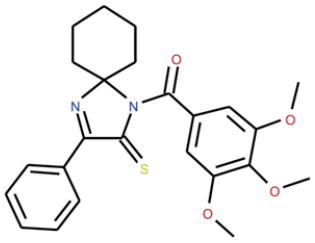
IC50 = 4.88 ± 0.4 µM
RelActDiff = 58 %
HillCoefficient = -3.0
ChiSquared = 3451.9
FitType = 4ParametersSigmoidal



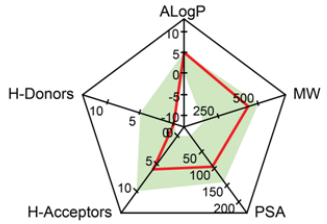
% Activity plotted against log conc. Dilutions of the compd (blue curve) with an integrated counter screen (green curve)

Chemical structure of the molecule

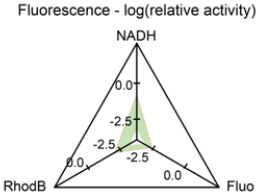
Similar chemical structures in this report:
212581,212579,212580,212575



212581



Red line: properties of the compd based on the molecular structure.
Shadowed area: ideal space of drug-like properties according to the Lipinski's rule (Rule of five).
MW: molecular weight.
H-Donors: number of hydrogen bind donors (OH, NH ..).
H-Acceptors: number of hydrogen bond acceptors (-O-, C=O ..).
ALogP: calculated distribution coefficient between water and octanol.



Red line: log relative activity of the compd measured at the wavelength of the references: 100µM NADH (340 nm) 0.1µM Fluorescein (495 nm) and 0.1µM Rhodamin B (560 nm).
Shadowed area determines the significance limit.

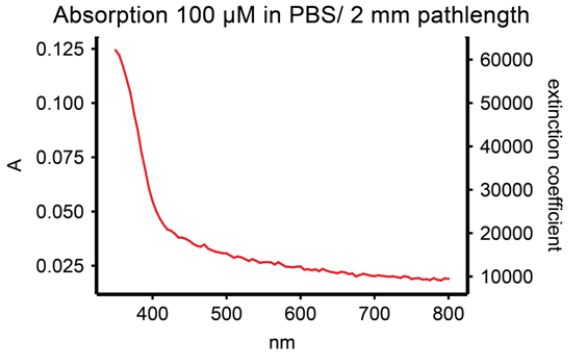
Statistical analysis of primary screens shows how often the compd was found in a specific screening technology (frequent hitter analysis).

Properties	Specificity
Solubility: Clear solution at 20 mM in DMSO: true Clear solution at 100 µM in aequeous PBS buffer: False Solubility in PBS/pH 7.5 between 12.3 and 16.0 µM Purity: PurityValue: 92.7 Comments: MeasurementDate: May 26, 2011 Fluorescence: 100uM NADH: 18.3% 0.1uM Fluorescein: 0.2% 0.1uM Rhodamin B: 0.8%	1 of 11 where redox_sensitive=false 0 of 5 where event_type=enzymeactivity 3 of 20 where biological=invitro 1 of 4 where assay_technology=elisa 3 of 13 where event_type=binding 1 of 4 where biological=cell 2 of 10 where redox_sensitive=true 2 of 7 where assay_technology=alphascreen 0 of 2 where assay_technology=LabChip 0 of 2 where event_type=phosphorylation 0 of 1 where assay_technology=FluoPol 0 of 1 where assay_technology=HTRF

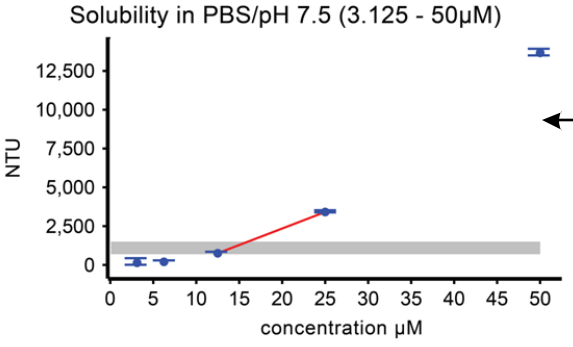
Solubility in DMSO by eye during the storage process.
Solubility in aqueous buffer according to a threshold value (> 2-fold higher than the buffer control) between 600-700 nm derived by the absorption graph below.
Solubility in PBS at pH 7.5 measured by nephelometry and derived by the graph to the right.
Purity value and its measurement date.
Determination of fluorescence in percent: 100% means fluorescent like the references.

Appearance 10 mM in DMSO

Picture of the compd solubilized in DMSO in the screening plate.



Absorption curve of the compd at 100 µM (absorption values between 600-700 nm (> 2-fold higher than buffer control) would define the compd as insoluble. Displayed in property table.



Green/Red dot: Decision wether the data is reliable (green) or not (red). based on solubility range (700 - 1500 NTU in grey).
The intersections of the red line with the upper and lower limit of the solubility range define the compd solubility. Displayed in property table.

Designed and developed by Dr. Martin Neuenschwander and Franziska Kreuchwig