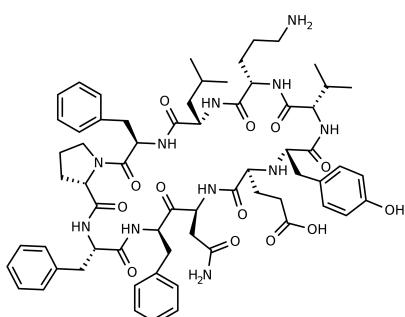


Figure 3-figure supplement 1

Tyrothricin Antibiotic

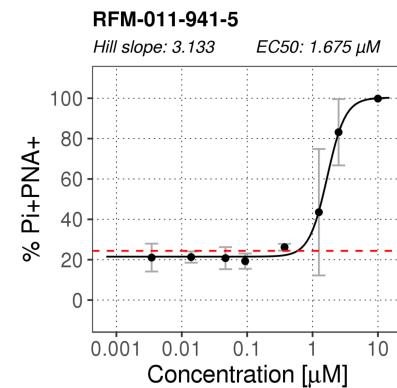


MW (RDKit)
1227.633

QED (RDKit)
0.063

SlogP (RDKit)
1.138

TPSA (RDKit)
379.75



EC50 [μ M]
1.67

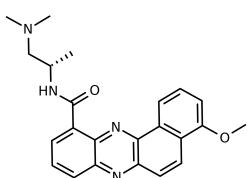
Efficacy [% induction]
84

Hek CC50 [μ M]
1.791

HepG2 CC50 [μ M]
0

MIn 576

DNA topoisomerase II inhibitor



MW (RDKit)
388.19

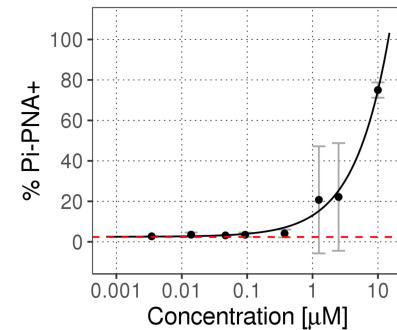
QED (RDKit)
0.418

SlogP (RDKit)
3.625

TPSA (RDKit)
67.35

RFM-008-110-7

Hill slope: 0.846 EC50: >10 μ M



EC50 [μ M]
>10

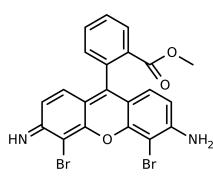
Efficacy [% induction]
76

Hek CC50 [μ M]
0.686

HepG2 CC50 [μ M]
0.574

Th-9402

Immunosuppressant



MW (RDKit)
499.937

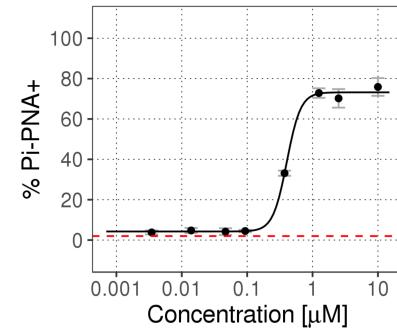
QED (RDKit)
0.213

SlogP (RDKit)
5.578

TPSA (RDKit)
89.31

RFM-006-521-4

Hill slope: 4.118 EC50: 0.404 μ M



EC50 [μ M]
0.4

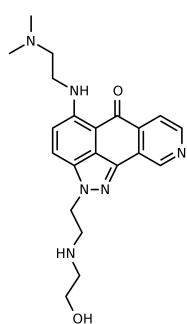
Efficacy [% induction]
76

Hek CC50 [μ M]
0

HepG2 CC50 [μ M]
0

Topixantrone

DNA topoisomerase II inhibitor



MW (RDKit)
394.212

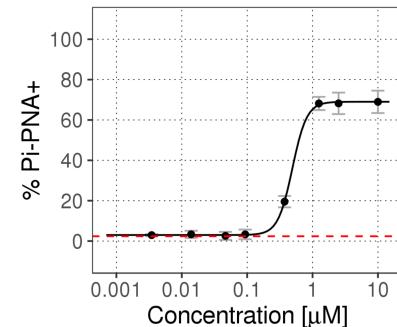
QED (RDKit)
0.367

SlogP (RDKit)
1.198

TPSA (RDKit)
95.31

RFM-009-126-9

Hill slope: 3.952 EC50: 0.491 μ M



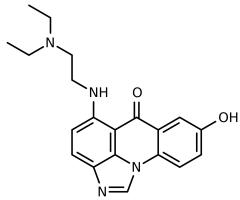
EC50 [μ M]
0.49

Efficacy [% induction]
72

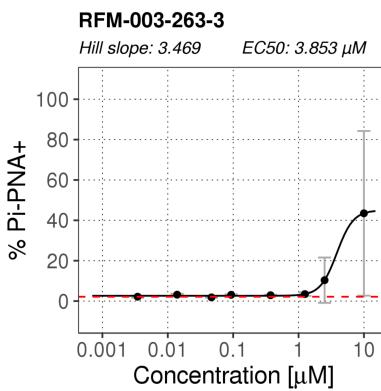
Hek CC50 [μ M]
1.443

HepG2 CC50 [μ M]
0.658

Imidazoacridinone
DNA topoisomerase II inhibitor

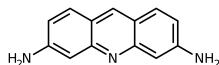


MW (RDKit) 350.174
QED (RDKit) 0.523
SlogP (RDKit) 2.898
TPSA (RDKit) 69.87

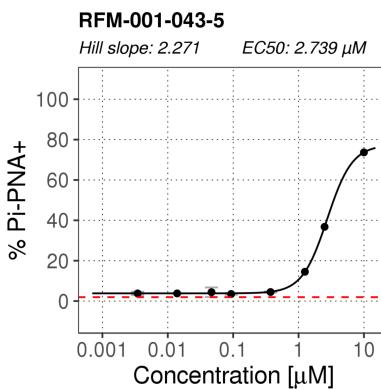


EC50 [μ M] 3.85
Efficacy [% induction] 71
Hek CC50 [μ M] 0.817
HepG2 CC50 [μ M] 0.476

Proflavine
DNA synthesis intercalator

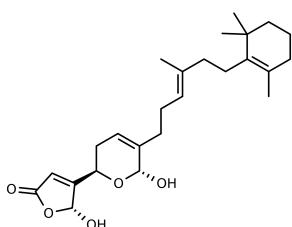


MW (RDKit) 209.095
QED (RDKit) 0.441
SlogP (RDKit) 2.552
TPSA (RDKit) 64.93

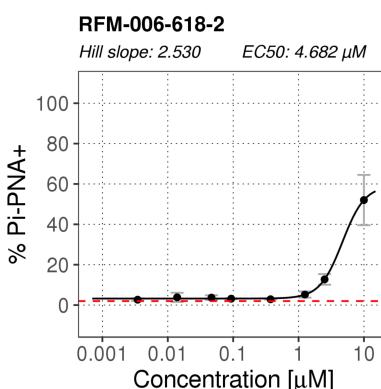


EC50 [μ M] 2.74
Efficacy [% induction] 71
Hek CC50 [μ M] 0
HepG2 CC50 [μ M] 0

Manoalide
Ornithine Decarboxylase/PLA2 inhibitor

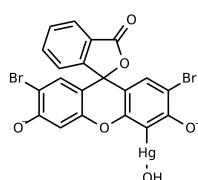


MW (RDKit) 416.256
QED (RDKit) 0.458
SlogP (RDKit) 4.855
TPSA (RDKit) 75.99

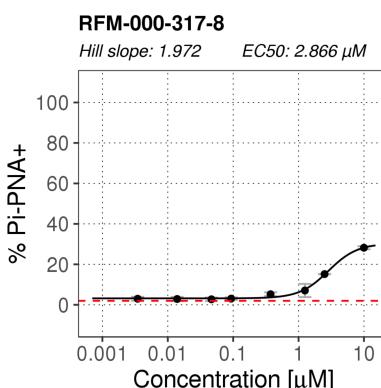


EC50 [μ M] 4.68
Efficacy [% induction] 59
Hek CC50 [μ M] 2.781
HepG2 CC50 [μ M] 3.522

Merbromin
Carbonic anhydrase II inhibitor

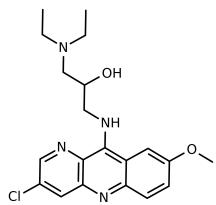


MW (RDKit) 703.841
QED (RDKit) 0.309
SlogP (RDKit) 2.542
TPSA (RDKit) 101.88



EC50 [μ M] 2.86
Efficacy [% induction] 27
Hek CC50 [μ M] 0
HepG2 CC50 [μ M] 0

Acranil
Antiprotozoal



MW (RDKit)

387.171

QED (RDKit)

0.568

SlogP (RDKit)

4.165

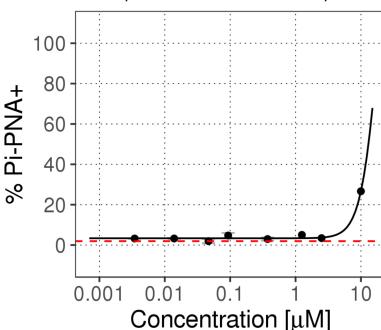
TPSA (RDKit)

57.62

RFM-000-968-7

Hill slope: 3.134

EC50: >10 μM



EC50 [μM]

>10

Efficacy [% induction]

25

Hek CC50 [μM]

1.136

HepG2 CC50 [μM]

2.827