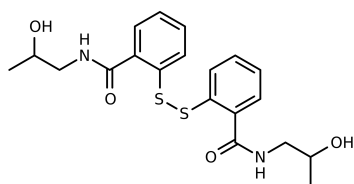


## Figure 2-figure supplement 1

### Kf-4939

Platelet aggregation inhibitor



**MW (RDKit)**  
420.118

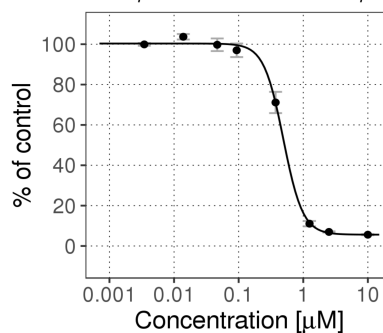
**QED (RDKit)**  
0.466

**SlogP (RDKit)**  
2.707

**TPSA (RDKit)**  
98.66

### RFM-007-885-3

Hill slope: -2.891 EC50: 0.491  $\mu$ M



**EC50 [μM]**  
0.49

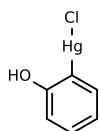
**Efficacy [% reduction]**  
100

**Hek CC50 [μM]**  
2.526

**HepG2 CC50 [μM]**  
0

### Mercufenol Chloride

Antiseptic



**MW (RDKit)**  
329.974

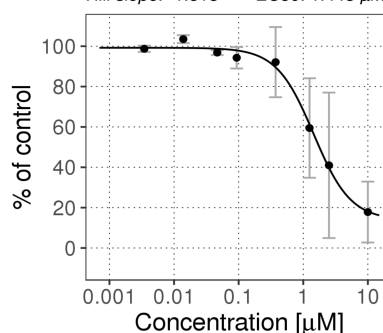
**QED (RDKit)**  
0.769

**SlogP (RDKit)**  
1.254

**TPSA (RDKit)**  
20.23

### RFM-006-841-7

Hill slope: -1.518 EC50: 1.448  $\mu$ M



**EC50 [μM]**  
1.45

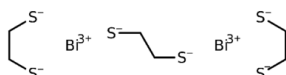
**Efficacy [% reduction]**  
98

**Hek CC50 [μM]**  
0.595

**HepG2 CC50 [μM]**  
2.721

### Bismuth Ethanedithiol

Unidentified pharmacological action



**MW (RDKit)**  
392.932

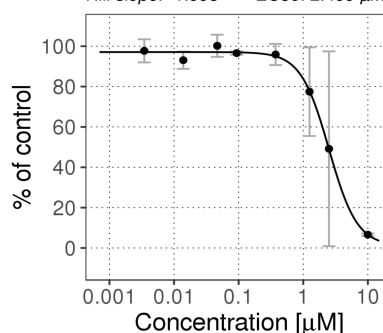
**QED (RDKit)**  
0.58

**SlogP (RDKit)**  
2.382

**TPSA (RDKit)**  
0

### RFM-011-751-1

Hill slope: -1.998 EC50: 2.499  $\mu$ M



**EC50 [μM]**  
2.5

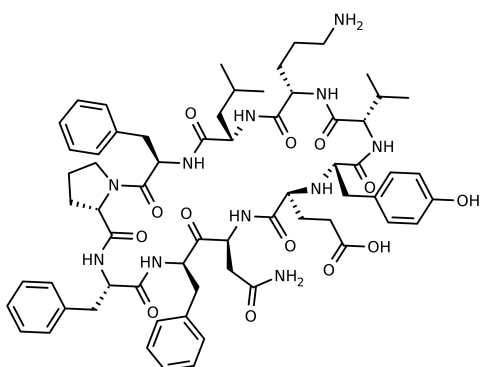
**Efficacy [% reduction]**  
98

**Hek CC50 [μM]**  
2.716

**HepG2 CC50 [μM]**  
1.141

### Tyrothricin

Antibiotic



**MW (RDKit)**  
1227.633

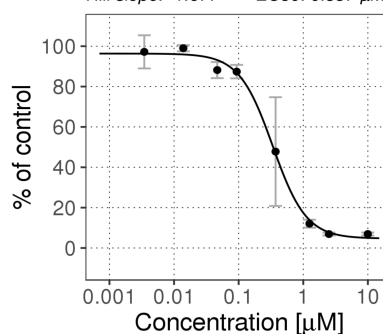
**QED (RDKit)**  
0.063

**SlogP (RDKit)**  
1.138

**TPSA (RDKit)**  
379.75

### RFM-011-941-5

Hill slope: -1.677 EC50: 0.337  $\mu$ M



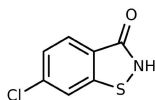
**EC50 [μM]**  
0.34

**Efficacy [% reduction]**  
97

**Hek CC50 [μM]**  
1.791

**HepG2 CC50 [μM]**  
0

**Ticlatone**  
Antibiotic

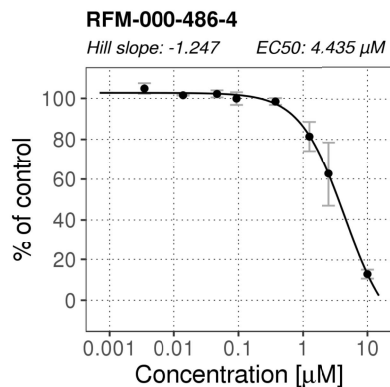


**MW (RDKit)**  
184.97

**QED (RDKit)**  
0.671

**SlogP (RDKit)**  
2.243

**TPSA (RDKit)**  
32.86



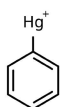
**EC50 [ $\mu$ M]**  
4.43

**Efficacy**  
[% reduction]  
96

**Hek CC50 [ $\mu$ M]**  
2.259

**HepG2 CC50 [ $\mu$ M]**  
0

**Phenylmercuric Borate**  
Antiseptic

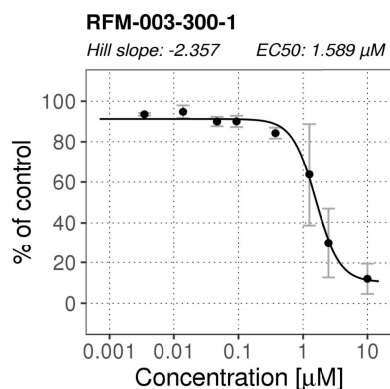


**MW (RDKit)**  
279.009

**QED (RDKit)**  
0.617

**SlogP (RDKit)**  
0.859

**TPSA (RDKit)**  
0



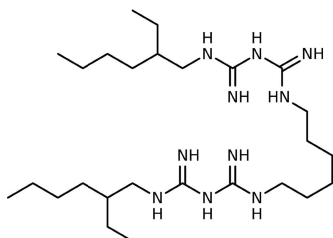
**EC50 [ $\mu$ M]**  
1.59

**Efficacy**  
[% reduction]  
91

**Hek CC50 [ $\mu$ M]**  
0.687

**HepG2 CC50 [ $\mu$ M]**  
0

**Alexidine**  
Phospholipase inhibitor

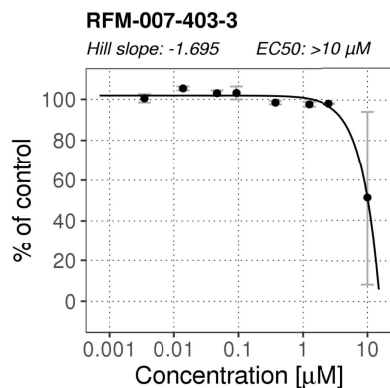


**MW (RDKit)**  
508.469

**QED (RDKit)**  
0.071

**SlogP (RDKit)**  
4.256

**TPSA (RDKit)**  
167.58



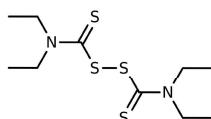
**EC50 [ $\mu$ M]**  
> 10

**Efficacy**  
[% reduction]  
86

**Hek CC50 [ $\mu$ M]**  
1.453

**HepG2 CC50 [ $\mu$ M]**  
1.506

**Disulfiram**  
Aldehyde dehydrogenase 2 inhibitor

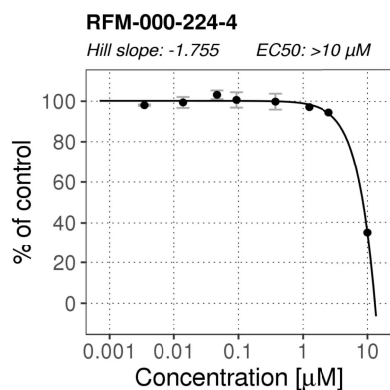


**MW (RDKit)**  
296.051

**QED (RDKit)**  
0.573

**SlogP (RDKit)**  
3.621

**TPSA (RDKit)**  
6.48



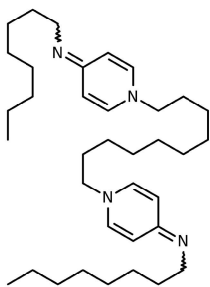
**EC50 [ $\mu$ M]**  
> 10

**Efficacy**  
[% reduction]  
70

**Hek CC50 [ $\mu$ M]**  
7.159

**HepG2 CC50 [ $\mu$ M]**  
0

**Octenidine**  
Antibacterial

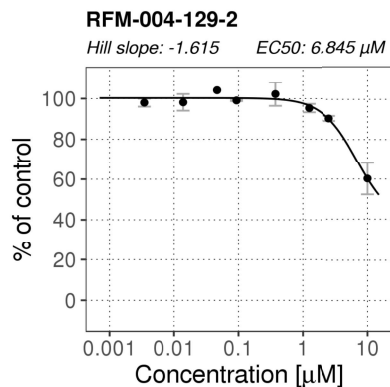


**MW (RDKit)**  
550.497

**QED (RDKit)**  
0.11

**SlogP (RDKit)**  
9.633

**TPSA (RDKit)**  
34.58



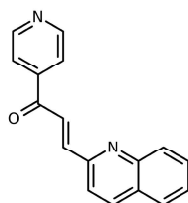
**$EC_{50}$  [ $\mu M$ ]**  
6.85

**Efficacy [% reduction]**  
54

**Hek CC50 [ $\mu M$ ]**  
0.798

**HepG2 CC50 [ $\mu M$ ]**  
1.763

**Pfk-015**  
PFKFB3 inhibitor

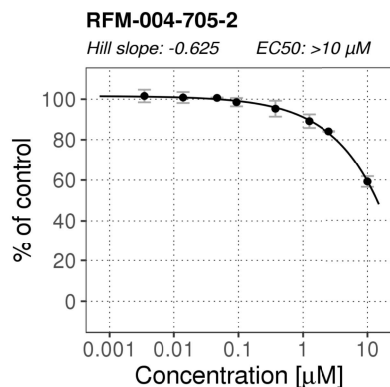


**MW (RDKit)**  
260.095

**QED (RDKit)**  
0.534

**SlogP (RDKit)**  
3.526

**TPSA (RDKit)**  
42.85



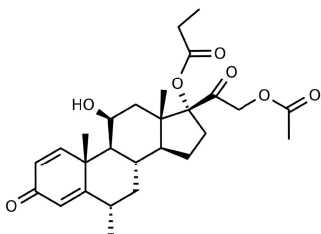
**$EC_{50}$  [ $\mu M$ ]**  
> 10

**Efficacy [% reduction]**  
47

**Hek CC50 [ $\mu M$ ]**  
1.382

**HepG2 CC50 [ $\mu M$ ]**  
0.95

**Methylprednisolone Aceponate**  
Antiinflammatory

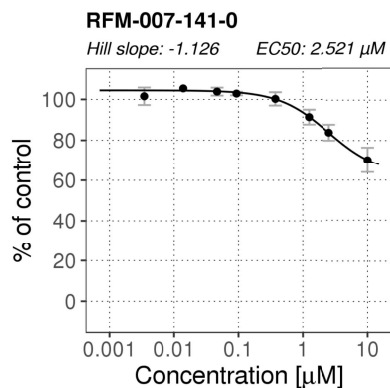


**MW (RDKit)**  
472.246

**QED (RDKit)**  
0.612

**SlogP (RDKit)**  
3.335

**TPSA (RDKit)**  
106.97



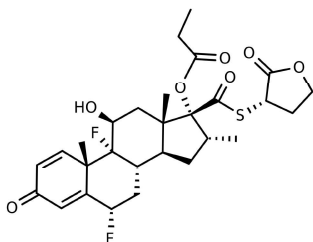
**$EC_{50}$  [ $\mu M$ ]**  
2.52

**Efficacy [% reduction]**  
45

**Hek CC50 [ $\mu M$ ]**  
0

**HepG2 CC50 [ $\mu M$ ]**  
0

**Zoticasone Propionate**  
Glucocorticoid receptor agonist

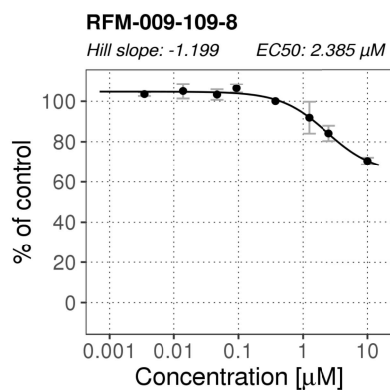


**MW (RDKit)**  
552.199

**QED (RDKit)**  
0.525

**SlogP (RDKit)**  
3.819

**TPSA (RDKit)**  
106.97



**$EC_{50}$  [ $\mu M$ ]**  
2.38

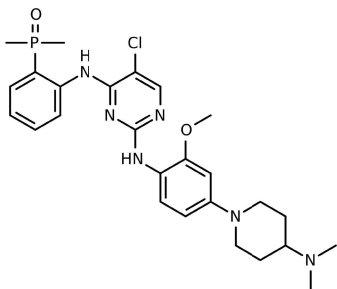
**Efficacy [% reduction]**  
39

**Hek CC50 [ $\mu M$ ]**  
0

**HepG2 CC50 [ $\mu M$ ]**  
0

### Brigatinib

ALK receptor tyrosine kinase inhibitor



MW (RDKit)  
528.217

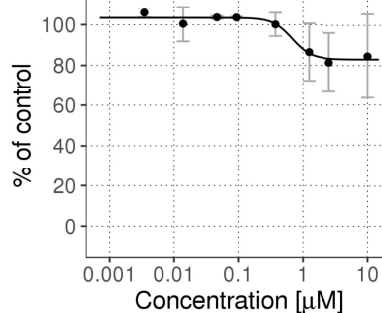
QED (RDKit)  
0.376

SlogP (RDKit)  
5.404

TPSA (RDKit)  
82.62

RFM-007-125-0

Hill slope: -2.921 EC50: 0.680  $\mu$ M



EC50 [ $\mu$ M]  
0.68

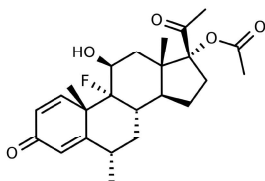
Efficacy  
[% reduction]  
38

Hek CC50 [ $\mu$ M]  
1.867

HepG2 CC50 [ $\mu$ M]  
0.136

### Fluorometholone Acetate

Antiinflammatory



MW (RDKit)  
418.216

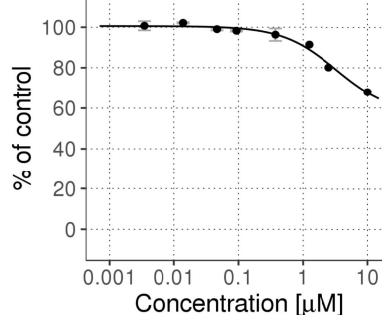
QED (RDKit)  
0.695

SlogP (RDKit)  
3.494

TPSA (RDKit)  
80.67

RFM-000-926-7

Hill slope: -1.038 EC50: 3.304  $\mu$ M



EC50 [ $\mu$ M]  
3.3

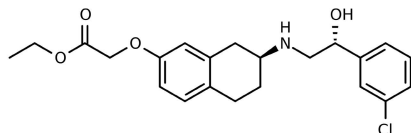
Efficacy  
[% reduction]  
35

Hek CC50 [ $\mu$ M]  
0

HepG2 CC50 [ $\mu$ M]  
0

### Amibegron Hydrochloride

beta3-Adrenoceptor Agonist



MW (RDKit)  
403.155

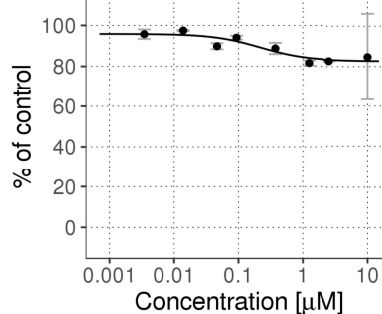
QED (RDKit)  
0.66

SlogP (RDKit)  
3.462

TPSA (RDKit)  
67.79

RFM-005-517-4

Hill slope: -1.170 EC50: 0.218  $\mu$ M



EC50 [ $\mu$ M]  
0.22

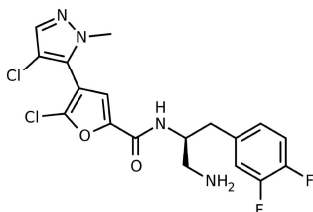
Efficacy  
[% reduction]  
31

Hek CC50 [ $\mu$ M]  
0

HepG2 CC50 [ $\mu$ M]  
0

### Uprosertib

PKB alpha/Akt1 inhibitor



MW (RDKit)  
428.062

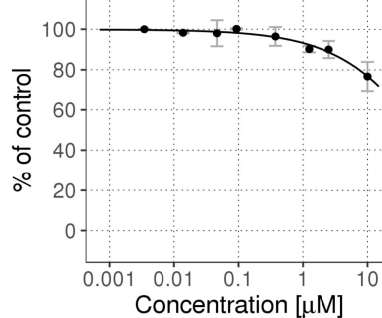
QED (RDKit)  
0.628

SlogP (RDKit)  
3.565

TPSA (RDKit)  
86.08

RFM-004-668-4

Hill slope: -0.595 EC50: >10  $\mu$ M



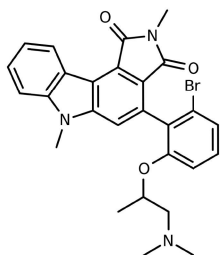
EC50 [ $\mu$ M]  
> 10

Efficacy  
[% reduction]  
31

Hek CC50 [ $\mu$ M]  
0

HepG2 CC50 [ $\mu$ M]  
0

**Kf-41399**  
Chemoprotective agent

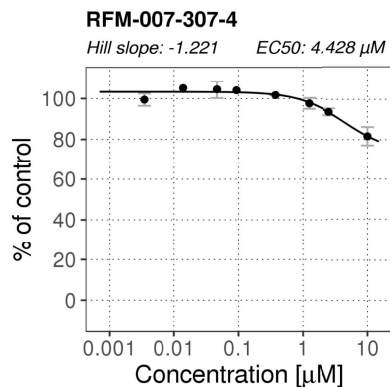


**MW (RDKit)**  
519.116

**QED (RDKit)**  
0.335

**SlogP (RDKit)**  
5.316

**TPSA (RDKit)**  
54.78



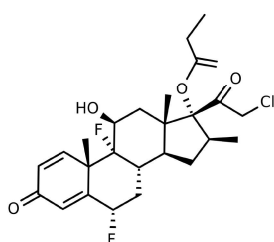
**EC50 [ $\mu\text{M}$ ]**  
4.43

**Efficacy [% reduction]**  
31

**Hek CC50 [ $\mu\text{M}$ ]**  
0

**HepG2 CC50 [ $\mu\text{M}$ ]**  
0

**Halobetasol Propionate**  
Antisporiatic

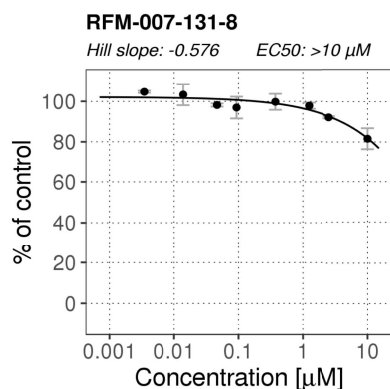


**MW (RDKit)**  
484.183

**QED (RDKit)**  
0.481

**SlogP (RDKit)**  
4.051

**TPSA (RDKit)**  
80.67



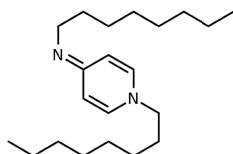
**EC50 [ $\mu\text{M}$ ]**  
> 10

**Efficacy [% reduction]**  
30

**Hek CC50 [ $\mu\text{M}$ ]**  
0

**HepG2 CC50 [ $\mu\text{M}$ ]**  
0

**Pirtenidine**  
Antibiotic

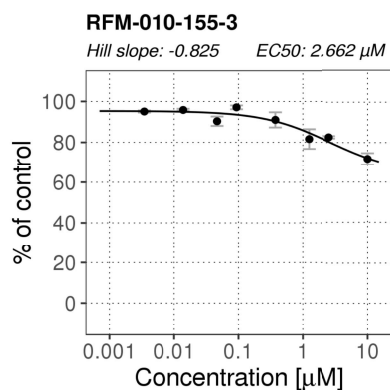


**MW (RDKit)**  
318.303

**QED (RDKit)**  
0.368

**SlogP (RDKit)**  
6.11

**TPSA (RDKit)**  
17.29



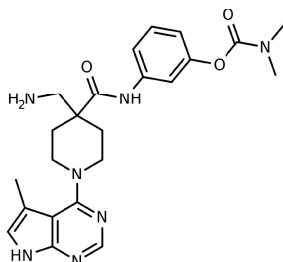
**EC50 [ $\mu\text{M}$ ]**  
2.66

**Efficacy [% reduction]**  
28

**Hek CC50 [ $\mu\text{M}$ ]**  
1.476

**HepG2 CC50 [ $\mu\text{M}$ ]**  
0

**Lx-7101**  
LIM Domain Kinase inhibitor

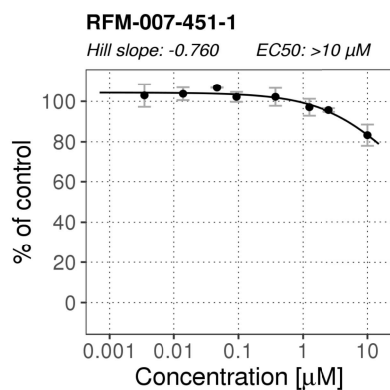


**MW (RDKit)**  
451.233

**QED (RDKit)**  
0.543

**SlogP (RDKit)**  
2.511

**TPSA (RDKit)**  
129.47



**EC50 [ $\mu\text{M}$ ]**  
> 10

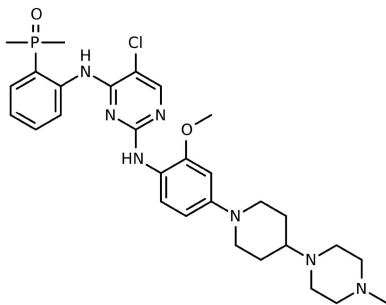
**Efficacy [% reduction]**  
28

**Hek CC50 [ $\mu\text{M}$ ]**  
0

**HepG2 CC50 [ $\mu\text{M}$ ]**  
0

### Ap26113-analog

ALK receptor tyrosine kinase inhibitor



MW (RDKit)  
528.217

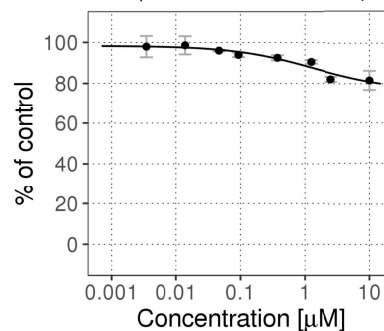
QED (RDKit)  
0.376

SlogP (RDKit)  
5.404

TPSA (RDKit)  
82.62

RFM-003-055-7

Hill slope: -0.695 EC50: 1.353  $\mu$ M



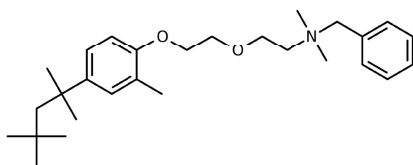
EC50 [μM]  
1.35

Efficacy  
[% reduction]  
24

Hek CC50 [μM]  
0

HepG2 CC50 [μM]  
0.13

### Methylbenzethonium Chloride Antiseptic



MW (RDKit)  
426.337

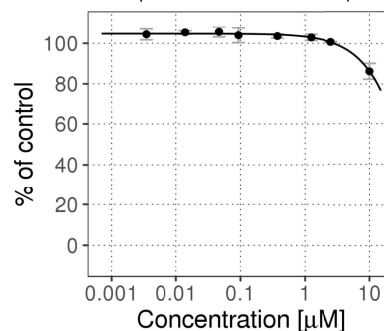
QED (RDKit)  
0.306

SlogP (RDKit)  
6.381

TPSA (RDKit)  
18.46

RFM-009-180-5

Hill slope: -1.134 EC50: >10  $\mu$ M



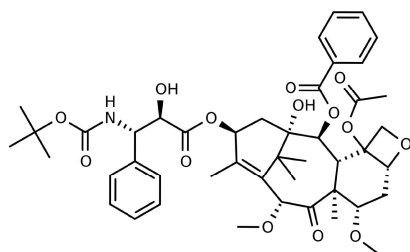
EC50 [μM]  
> 10

Efficacy  
[% reduction]  
24

Hek CC50 [μM]  
3.65

HepG2 CC50 [μM]  
7.586

### Cabazitaxel Tubulin inhibitor



MW (RDKit)  
835.378

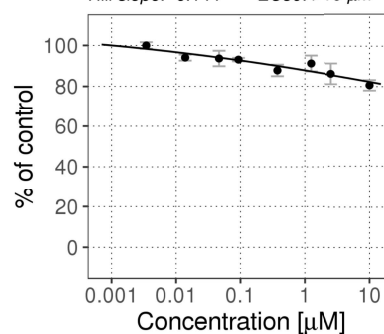
QED (RDKit)  
0.171

SlogP (RDKit)  
4.568

TPSA (RDKit)  
202.45

RFM-003-386-3

Hill slope: -0.144 EC50: >10  $\mu$ M



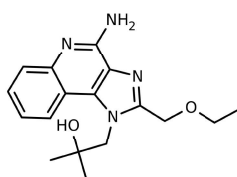
EC50 [μM]  
> 10

Efficacy  
[% reduction]  
23

Hek CC50 [μM]  
0

HepG2 CC50 [μM]  
0

### Resiquimod Immunostimulant



MW (RDKit)  
314.174

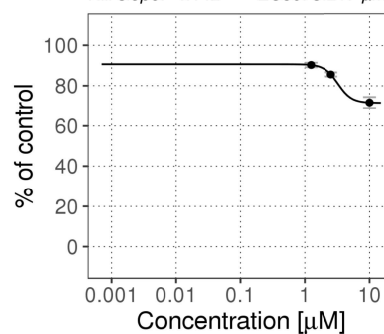
QED (RDKit)  
0.755

SlogP (RDKit)  
2.474

TPSA (RDKit)  
86.19

RFM-004-547-6

Hill slope: -4.142 EC50: 3.217  $\mu$ M



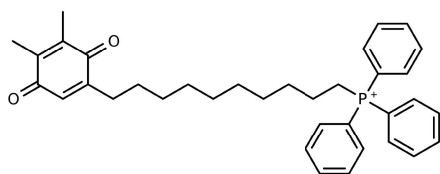
EC50 [μM]  
3.22

Efficacy  
[% reduction]  
22

Hek CC50 [μM]  
0

HepG2 CC50 [μM]  
0

**Skq1**  
Neurologic drug

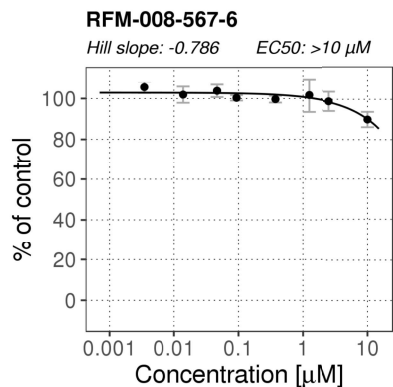


**MW (RDKit)**  
537.292

**QED (RDKit)**  
0.119

**SlogP (RDKit)**  
7.906

**TPSA (RDKit)**  
34.14



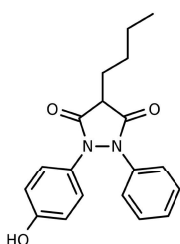
**EC50 [ $\mu\text{M}$ ]**  
> 10

**Efficacy [% reduction]**  
21

**Hek CC50 [ $\mu\text{M}$ ]**  
0.778

**HepG2 CC50 [ $\mu\text{M}$ ]**  
4.41

**Oxyphenbutazone**  
Treatment of Gout

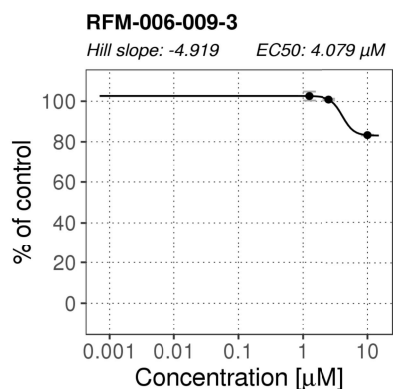


**MW (RDKit)**  
324.147

**QED (RDKit)**  
0.856

**SlogP (RDKit)**  
3.493

**TPSA (RDKit)**  
60.85



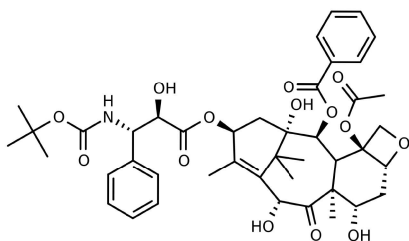
**EC50 [ $\mu\text{M}$ ]**  
4.08

**Efficacy [% reduction]**  
21

**Hek CC50 [ $\mu\text{M}$ ]**  
1.572

**HepG2 CC50 [ $\mu\text{M}$ ]**  
0

**Docetaxel**  
Tubulin inhibitor

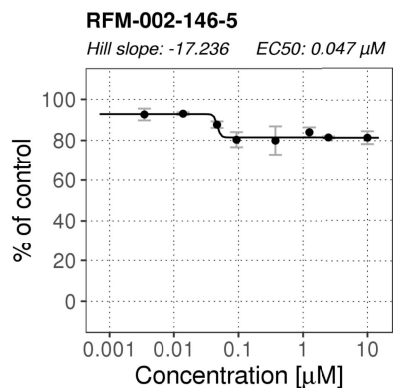


**MW (RDKit)**  
807.347

**QED (RDKit)**  
0.147

**SlogP (RDKit)**  
3.26

**TPSA (RDKit)**  
224.45



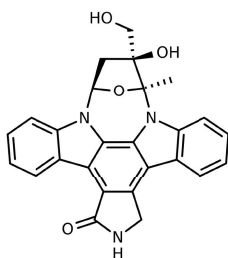
**EC50 [ $\mu\text{M}$ ]**  
0.05

**Efficacy [% reduction]**  
20

**Hek CC50 [ $\mu\text{M}$ ]**  
0

**HepG2 CC50 [ $\mu\text{M}$ ]**  
0

**Lestaurtinib**  
Flt3 inhibitor

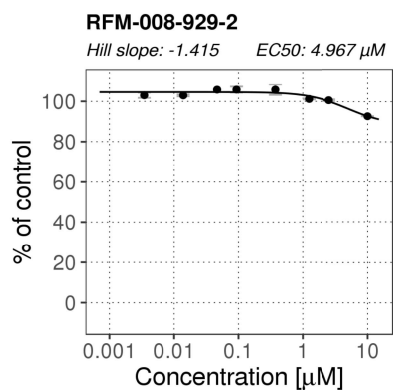


**MW (RDKit)**  
439.153

**QED (RDKit)**  
0.373

**SlogP (RDKit)**  
3.474

**TPSA (RDKit)**  
88.65



**EC50 [ $\mu\text{M}$ ]**  
4.97

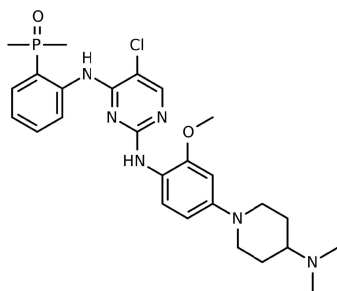
**Efficacy [% reduction]**  
17

**Hek CC50 [ $\mu\text{M}$ ]**  
0.551

**HepG2 CC50 [ $\mu\text{M}$ ]**  
0.029

## Brigatinib

ALK receptor tyrosine kinase inhibitor

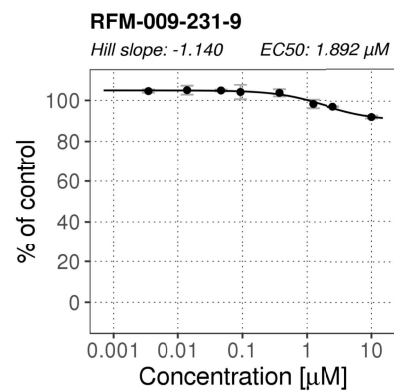


**MW (RDKit)**  
583.259

**QED (RDKit)**  
0.352

**SlogP (RDKit)**  
5.09

**TPSA (RDKit)**  
85.86



**EC50 [ $\mu\text{M}$ ]**  
1.89

**Efficacy**  
[% reduction]  
15

**Hek CC50 [ $\mu\text{M}$ ]**  
8.066

**HepG2 CC50 [ $\mu\text{M}$ ]**  
0.435