SUPPLEMENTAL FILES

Design and in silico study of the novel coumarin derivatives against SARS-CoV-2 main enzymes.

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Predicted Pharmacokinetic Properties (ADMET) Properties of Coumarins (1-17) by pkCSM.

- For 7-hydroxy-4,8-dimethyl-3-propanoate coumarin (1)

| Molecule Depiction | Molecule Properties |
|--------------------|---------------------|
| Descriptor         | Value               |
| Molecular Weight   | 308.333 g/mol       |
| LogP              | 3.6096              |
| #Rotatable Bonds   | 4                   |
| #Acceptors        | 4                   |
| #Donors           | 1                   |
| Surface Area      | 132.552             |

| Property            | Model Name                  | Value | Unit                  |
|---------------------|-----------------------------|-------|-----------------------|
| Absorption          | Water solubility            | -4.296| Numeric (log mol/L)   |
| Absorption          | Caco2 permeability          | 0.955 | Numeric (log Papp in 10^-6 cm/s) |
| Absorption          | Intestinal absorption (human)| 96.137| Numeric (% Absorbed)  |
| Absorption          | Skin Permeability           | -2.787| Numeric (log Kp)      |
| Absorption          | P-glycoprotein substrate    | No    | Categorical (Yes/No)  |
| Absorption          | P-glycoprotein I inhibitor  | No    | Categorical (Yes/No)  |
| Absorption          | P-glycoprotein II inhibitor | Yes   | Categorical (Yes/No)  |
| Distribution        | VDss (human)                | -0.137| Numeric (log L/kg)    |
| Distribution        | Fraction unbound (human)    | 0.075 | Numeric (Fu)          |
| Distribution        | BBB permeability            | -0.14 | Numeric (log BB)      |
| Distribution        | CNS permeability            | -2.059| Numeric (log PS)      |
| Metabolism          | CYP2D6 substrate            | No    | Categorical (Yes/No)  |
| Metabolism          | CYP3A4 substrate            | Yes   | Categorical (Yes/No)  |
| Metabolism          | CYP1A2 inhibitor            | Yes   | Categorical (Yes/No)  |
| Metabolism          | CYP2C19 inhibitor           | Yes   | Categorical (Yes/No)  |
| Metabolism          | CYP2C9 inhibitor            | Yes   | Categorical (Yes/No)  |
| Metabolism          | CYP2D6 inhibitor            | No    | Categorical (Yes/No)  |
| Metabolism          | CYP3A4 inhibitor            | Yes   | Categorical (Yes/No)  |
| Excretion           | Total Clearance             | 0.803 | Numeric (log ml/min/kg) |
| Excretion           | Renal OCT2 substrate       | No    | Categorical (Yes/No)  |
| Toxicity            | AMES toxicity               | No    | Categorical (Yes/No)  |
| Toxicity            | Max. tolerated dose (human) | 0.289 | Numeric (log mg/kg/day) |
| Toxicity            | hERG I inhibitor            | No    | Categorical (Yes/No)  |
| Toxicity            | hERG II inhibitor           | Yes   | Categorical (Yes/No)  |
| Toxicity            | Oral Rat Acute Toxicity (LD50)| 2.568| Numeric (mol/kg)    |
| Toxicity            | Oral Rat Chronic Toxicity (LOAEL) | 1.593| Numeric (log mg/kg_bw/day) |
| Toxicity            | Hepatotoxicity             | Yes   | Categorical (Yes/No)  |
| Toxicity            | Skin Sensitisation         | No    | Categorical (Yes/No)  |
| Toxicity            | T.Pyformis toxicity        | 0.573 | Numeric (log ug/L)    |
| Toxicity            | Minnow toxicity            | -0.029| Numeric (log mM)      |
For 7-hydroxy-4,8-dimethyl-3-propanamide coumarin (2)

| Molecule Properties | Molecule Depiction |
|---------------------|--------------------|
| Descriptor          | Value              |
| Molecular Weight    | 332.4 g/mol        |
| LogP                | 1.72584            |
| #Rotatable Bonds    | 6                  |
| #Acceptors          | 5                  |
| #Donors             | 2                  |
| Surface Area        | 140.629            |

| Property                      | Model Name         | Value                      | Unit                      |
|-------------------------------|--------------------|----------------------------|---------------------------|
| Absorption Water solubility  | -3.212             | Numeric (log mol/L)        |
| Absorption Caco2 permeability| 0.553              | Numeric (log Papp in 10^{-6} cm/s) |
| Absorption Intestinal absorption (human) | 95.212 | Numeric (% Absorbed) |
| Absorption Skin Permeability | -3.54              | Numeric (log Kp)           |
| Absorption P-glycoprotein substrate | Yes | Categorical (Yes/No) |
| Absorption P-glycoprotein I inhibitor | No | Categorical (Yes/No) |
| Absorption P-glycoprotein II inhibitor | No | Categorical (Yes/No) |
| Distribution VDss (human)    | 0.935              | Numeric (log L/kg)         |
| Distribution Fraction unbound (human) | 0.362 | Numeric (Fu) |
| Distribution BBB permeability| -0.895             | Numeric (log BB)           |
| Distribution CNS permeability| -2.774             | Numeric (log PS)           |
| Metabolism CYP2D6 substrate  | No                 | Categorical (Yes/No)      |
| Metabolism CYP3A4 substrate  | Yes                | Categorical (Yes/No)      |
| Metabolism CYP1A2 inhibitor  | Yes                | Categorical (Yes/No)      |
| Metabolism CYP2C19 inhibitor  | No                 | Categorical (Yes/No)      |
| Metabolism CYP2C9 inhibitor  | No                 | Categorical (Yes/No)      |
| Metabolism CYP2D6 inhibitor  | No                 | Categorical (Yes/No)      |
| Metabolism CYP3A4 inhibitor  | No                 | Categorical (Yes/No)      |
| Excretion Total Clearance    | 0.786              | Numeric (log ml/min/kg)    |
| Excretion Renal OCT2 substrate| No                 | Categorical (Yes/No)      |
| Toxicity AMES toxicity       | No                 | Categorical (Yes/No)      |
| Toxicity Max. tolerated dose (human) | 0.109 | Numeric (log mg/kg/day) |
| Toxicity hERG I inhibitor    | No                 | Categorical (Yes/No)      |
| Toxicity hERG II inhibitor   | Yes                | Categorical (Yes/No)      |
| Toxicity Oral Rat Acute Toxicity (LD50) | 2.534 | Numeric (mol/kg) |
| Toxicity Oral Rat Chronic Toxicity (LOAEL) | 0.942 | Numeric (log mg/kg_bw/day) |
| Toxicity Hepatotoxicity      | Yes                | Categorical (Yes/No)      |
| Toxicity Skin Sensitisation  | No                 | Categorical (Yes/No)      |
| Toxicity T. Pyriformis toxicity | 1.057 | Numeric (log ug/L) |
| Toxicity Minnow toxicity     | 2.977              | Numeric (log mM)           |
For 7-hydroxy-4,8-dimethyl-3-N-(2-morphinoethyl)propanamide coumarin (3)

| Molecule Properties | Descriptor               | Value           |
|---------------------|--------------------------|-----------------|
| Molecular Weight    |                          | 374.437 g/mol   |
| LogP               |                          | 1.49644         |
| #Rotatable Bonds    |                          | 6               |
| #Acceptors         |                          | 6               |
| #Donors            |                          | 2               |
| Surface Area       |                          | 157.467         |

**Property** | **Model Name** | **Value** | **Unit**  
---|---|---|---|
**Absorption** | Water solubility | -2.733 | Numeric (log mol/L) |
**Absorption** | Caco2 permeability | 0.008 | Numeric (log Papp in 10⁻⁶ cm/s) |
**Absorption** | Intestinal absorption (human) | 75.682 | Numeric (% Absorbed) |
**Absorption** | Skin Permeability | -2.954 | Numeric (log Kp) |
**Absorption** | P-glycoprotein substrate | Yes | Categorical (Yes/No) |
**Absorption** | P-glycoprotein I inhibitor | Yes | Categorical (Yes/No) |
**Absorption** | P-glycoprotein II inhibitor | No | Categorical (Yes/No) |
**Distribution** | VDss (human) | 1.175 | Numeric (log L/kg) |
**Distribution** | Fraction unbound (human) | 0.36 | Numeric (Fu) |
**Distribution** | BBB permeability | -0.649 | Numeric (log BB) |
**Distribution** | CNS permeability | -2.901 | Numeric (log PS) |
**Metabolism** | CYP2D6 substrate | No | Categorical (Yes/No) |
**Metabolism** | CYP3A4 substrate | Yes | Categorical (Yes/No) |
**Metabolism** | CYP1A2 inhibitor | No | Categorical (Yes/No) |
**Metabolism** | CYP2C19 inhibitor | No | Categorical (Yes/No) |
**Metabolism** | CYP2C9 inhibitor | No | Categorical (Yes/No) |
**Metabolism** | CYP2D6 inhibitor | No | Categorical (Yes/No) |
**Metabolism** | CYP3A4 inhibitor | No | Categorical (Yes/No) |
**Excretion** | Total Clearance | 1.014 | Numeric (log ml/min/kg) |
**Excretion** | Renal OCT2 substrate | Yes | Categorical (Yes/No) |
**Toxicity** | AMES toxicity | No | Categorical (Yes/No) |
**Toxicity** | Max. tolerated dose (human) | -0.298 | Numeric (log mg/kg/day) |
**Toxicity** | hERG I inhibitor | No | Categorical (Yes/No) |
**Toxicity** | hERG II inhibitor | Yes | Categorical (Yes/No) |
**Toxicity** | Oral Rat Acute Toxicity (LD50) | 2.081 | Numeric (mol/kg) |
**Toxicity** | Oral Rat Chronic Toxicity (LOAEL) | 1.785 | Numeric (log mg/kg_bw/day) |
**Toxicity** | Hepatotoxicity | Yes | Categorical (Yes/No) |
**Toxicity** | Skin Sensitisation | No | Categorical (Yes/No) |
**Toxicity** | T. Pyriformis toxicity | 0.512 | Numeric (log ug/L) |
**Toxicity** | Minnow toxicity | 1.728 | Numeric (log mM) |
- For 7-hydroxy-4,8-dimethyl-3-N-(2-piperidin-1-yl)ethyl)propanamide coumarin (4)

| Property | Model Name | Value | Unit |
|----------|------------|-------|------|
| Absorption | Water solubility | -3.142 | Numeric (log mol/L) |
| Absorption | Caco2 permeability | 1.061 | Numeric (log Papp in 10^-6 cm/s) |
| Absorption | Intestinal absorption (human) | 93.426 | Numeric (% Absorbed) |
| Absorption | Skin Permeability | -2.957 | Numeric (log Kp) |
| Absorption | P-glycoprotein substrate | Yes | Categorical (Yes/No) |
| Absorption | P-glycoprotein I inhibitor | Yes | Categorical (Yes/No) |
| Absorption | P-glycoprotein II inhibitor | Yes | Categorical (Yes/No) |
| Distribution | VDss (human) | 1.467 | Numeric (log L/kg) |
| Distribution | Fraction unbound (human) | 0.317 | Numeric (Fu) |
| Distribution | BBB permeability | -0.576 | Numeric (log BB) |
| Distribution | CNS permeability | -2.569 | Numeric (log PS) |
| Metabolism | CYP2D6 substrate | No | Categorical (Yes/No) |
| Metabolism | CYP3A4 substrate | Yes | Categorical (Yes/No) |
| Metabolism | CYP1A2 inhibitor | No | Categorical (Yes/No) |
| Metabolism | CYP2C19 inhibitor | No | Categorical (Yes/No) |
| Metabolism | CYP2C9 inhibitor | No | Categorical (Yes/No) |
| Metabolism | CYP2D6 inhibitor | Yes | Categorical (Yes/No) |
| Metabolism | CYP3A4 inhibitor | No | Categorical (Yes/No) |
| Excretion | Total Clearance | 0.972 | Numeric (log ml/min/kg) |
| Excretion | Renal OCT2 substrate | Yes | Categorical (Yes/No) |
| Toxicity | AMES toxicity | No | Categorical (Yes/No) |
| Toxicity | Max. tolerated dose (human) | -0.326 | Numeric (log mg/kg/day) |
| Toxicity | hERG I inhibitor | No | Categorical (Yes/No) |
| Toxicity | hERG II inhibitor | Yes | Categorical (Yes/No) |
| Toxicity | Oral Rat Acute Toxicity (LD50) | 2.378 | Numeric (mol/kg) |
| Toxicity | Oral Rat Chronic Toxicity (LOAEL) | 1.486 | Numeric (log mg/kg bw/day) |
| Toxicity | Hepatotoxicity | Yes | Categorical (Yes/No) |
| Toxicity | Skin Sensitisation | No | Categorical (Yes/No) |
| Toxicity | T. Pyriformis toxicity | 0.58 | Numeric (log ug/L) |
| Toxicity | Minnow toxicity | 1.572 | Numeric (log mM) |
For 7-hydroxy-4,8-dimethyl-3-N-(2-(piperazin-1-yl)ethyl)propanamide coumarin (5)

| Molecule Depiction | Molecule Properties |
|--------------------|---------------------|
| ![Molecule](image) | Descriptor | Value |
| | Molecular Weight | 373.453 g/mol |
| | LogP | 1.06944 |
| | #Rotatable Bonds | 6 |
| | #Acceptors | 6 |
| | #Donors | 3 |
| | Surface Area | 157.903 |

| Property | Model Name | Value | Unit |
|----------|------------|-------|------|
| Absorption | Water solubility | -2.429 | Numeric (log mol/L) |
| Absorption | Caco2 permeability | -0.078 | Numeric (log Papp in 10^(-6) cm/s) |
| Absorption | Intestinal absorption (human) | 66.482 | Numeric (% Absorbed) |
| Absorption | Skin Permeability | -2.765 | Numeric (log Kp) |
| Absorption | P-glycoprotein substrate | Yes | Categorical (Yes/No) |
| Absorption | P-glycoprotein I inhibitor | No | Categorical (Yes/No) |
| Absorption | P-glycoprotein II inhibitor | No | Categorical (Yes/No) |
| Distribution | VDss (human) | 1.821 | Numeric (log L/kg) |
| Distribution | Fraction unbound (human) | 0.42 | Numeric (Fu) |
| Distribution | BBB permeability | -0.628 | Numeric (log BB) |
| Distribution | CNS permeability | -2.979 | Numeric (log PS) |
| Metabolism | CYP2D6 substrate | No | Categorical (Yes/No) |
| Metabolism | CYP3A4 substrate | Yes | Categorical (Yes/No) |
| Metabolism | CYP1A2 inhibitor | No | Categorical (Yes/No) |
| Metabolism | CYP2C19 inhibitor | No | Categorical (Yes/No) |
| Metabolism | CYP2C9 inhibitor | No | Categorical (Yes/No) |
| Metabolism | CYP2D6 inhibitor | No | Categorical (Yes/No) |
| Metabolism | CYP3A4 inhibitor | No | Categorical (Yes/No) |
| Excretion | Total Clearance | 0.91 | Numeric (log ml/min/kg) |
| Excretion | Renal OCT2 substrate | No | Categorical (Yes/No) |
| Toxicity | AMES toxicity | No | Categorical (Yes/No) |
| Toxicity | Max. tolerated dose (human) | -0.253 | Numeric (log mg/kg/day) |
| Toxicity | hERG I inhibitor | No | Categorical (Yes/No) |
| Toxicity | hERG II inhibitor | Yes | Categorical (Yes/No) |
| Toxicity | Oral Rat Acute Toxicity (LD50) | 2.269 | Numeric (mol/kg) |
| Toxicity | Oral Rat Chronic Toxicity (LOAEL) | 2.279 | Numeric (log mg/kg bw/day) |
| Toxicity | Hepatotoxicity | Yes | Categorical (Yes/No) |
| Toxicity | Skin Sensitisation | No | Categorical (Yes/No) |
| Toxicity | T.Pyrophorus toxicity | 0.339 | Numeric (log ug/L) |
| Toxicity | Minnow toxicity | 2.834 | Numeric (log mM) |
For 7-hydroxy-4,8-dimethyl-3-N-propylpropanamide coumarin (6)

![Molecule Depiction](image)

| Molecule Properties | Value |
|---------------------|-------|
| Molecular Weight    | 303.358 g/mol |
| LogP               | 2.575424 |
| #Rotatable Bonds    | 5 |
| #Acceptors         | 4 |
| #Donors            | 2 |
| Surface Area       | 128.505 |

| Property                              | Model Name                     | Value | Unit                  |
|---------------------------------------|--------------------------------|-------|-----------------------|
| Absorption                           | Water solubility               | -3.84 | Numeric (log mol/L)  |
| Absorption                           | Caco2 permeability             | 1.174 | Numeric (log Papp in 10^{-6} cm/s) |
| Absorption                           | Intestinal absorption (human)  | 94.69 | Numeric (% Absorbed)  |
| Absorption                           | Skin Permeability              | -3.408 | Numeric (log Kp) |
| Absorption                           | P-glycoprotein substrate       | Yes   | Categorical (Yes/No)  |
| Absorption                           | P-glycoprotein I inhibitor     | No    | Categorical (Yes/No)  |
| Absorption                           | P-glycoprotein II inhibitor    | No    | Categorical (Yes/No)  |
| Distribution                         | VDss (human)                   | 0.319 | Numeric (log L/kg)    |
| Distribution                         | Fraction unbound (human)       | 0.223 | Numeric (Fu)          |
| Distribution                         | BBB permeability               | -0.273 | Numeric (log BB)     |
| Distribution                         | CNS permeability               | -2.454 | Numeric (log PS)     |
| Metabolism                           | CYP2D6 substrate              | No    | Categorical (Yes/No)  |
| Metabolism                           | CYP3A4 substrate              | Yes   | Categorical (Yes/No)  |
| Metabolism                           | CYP1A2 inhibitor               | Yes   | Categorical (Yes/No)  |
| Metabolism                           | CYP2C19 inhibitor              | No    | Categorical (Yes/No)  |
| Metabolism                           | CYP2C9 inhibitor               | No    | Categorical (Yes/No)  |
| Metabolism                           | CYP2D6 inhibitor               | No    | Categorical (Yes/No)  |
| Metabolism                           | CYP3A4 inhibitor               | No    | Categorical (Yes/No)  |
| Excretion                            | Total Clearance                | 1.022 | Numeric (log ml/min/kg) |
| Excretion                            | Renal OCT2 substrate          | No    | Categorical (Yes/No)  |
| Toxicity                             | AMES toxicity                  | Yes   | Categorical (Yes/No)  |
| Toxicity                             | Max. tolerated dose (human)    | 0.302 | Numeric (log mg/kg/day) |
| Toxicity                             | hERG I inhibitor               | No    | Categorical (Yes/No)  |
| Toxicity                             | hERG II inhibitor              | No    | Categorical (Yes/No)  |
| Toxicity                             | Oral Rat Acute Toxicity (LD50) | 2.471 | Numeric (mol/kg)      |
| Toxicity                             | Oral Rat Chronic Toxicity (LOAEL) | 0.908 | Numeric (log mg/kg_bw/day) |
| Toxicity                             | Hepatotoxicity                 | Yes   | Categorical (Yes/No)  |
| Toxicity                             | Skin Sensitisation             | No    | Categorical (Yes/No)  |
| Toxicity                             | T.Pyreiformis toxicity         | 1.422 | Numeric (log ug/L)    |
| Toxicity                             | Minnow toxicity                | 1.309 | Numeric (log mM)      |
For 7-hydroxy-4,8-dimethyl-3-N-phenylpropanamide coumarin (7)

### Molecule Depiction

![Molecule Depiction](image)

### Molecule Properties

| Descriptor                  | Value       |
|-----------------------------|-------------|
| Molecular Weight            | 337.375 g/mol |
| LogP                        | 3.68674     |
| #Rotatable Bonds            | 4           |
| #Acceptors                  | 4           |
| #Donors                     | 2           |
| Surface Area                | 144.467     |

### Property Model Name Value Unit

| Property                                | Model Name         | Value     | Unit                  |
|-----------------------------------------|--------------------|-----------|-----------------------|
| Absorption Water solubility             |                    | -4.423    | Numeric (log mol/L)   |
| Absorption Caco2 permeability           |                    | 1.041     | Numeric (log Papp in 10^-6 cm/s) |
| Absorption Intestinal absorption (human)|                    | 91.427    | Numeric (% Absorbed)  |
| Absorption Skin Permeability            |                    | -2.822    | Numeric (log Kp)      |
| Absorption P-glycoprotein substrate     |                    | Yes       | Categorical (Yes/No)  |
| Absorption P-glycoprotein I inhibitor   |                    | Yes       | Categorical (Yes/No)  |
| Absorption P-glycoprotein II inhibitor  |                    | Yes       | Categorical (Yes/No)  |
| Distribution VDss (human)               |                    | -0.258    | Numeric (log L/kg)    |
| Distribution Fraction unbound (human)   |                    | 0         | Numeric (Fu)          |
| Distribution BBB permeability           |                    | 0.043     | Numeric (log BB)      |
| Distribution CNS permeability           |                    | -2.016    | Numeric (log PS)      |
| Metabolism CYP2D6 substrate             |                    | No        | Categorical (Yes/No)  |
| Metabolism CYP3A4 substrate             |                    | Yes       | Categorical (Yes/No)  |
| Metabolism CYP1A2 inhibitor             |                    | Yes       | Categorical (Yes/No)  |
| Metabolism CYP2C19 inhibitor            |                    | Yes       | Categorical (Yes/No)  |
| Metabolism CYP2C9 inhibitor             |                    | Yes       | Categorical (Yes/No)  |
| Metabolism CYP2D6 inhibitor             |                    | No        | Categorical (Yes/No)  |
| Metabolism CYP3A4 inhibitor             |                    | Yes       | Categorical (Yes/No)  |
| Excretion Total Clearance               |                    | 0.729     | Numeric (log ml/min/kg) |
| Excretion Renal OCT2 substrate          |                    | No        | Categorical (Yes/No)  |
| Toxicity AMES toxicity                  |                    | No        | Categorical (Yes/No)  |
| Toxicity Max. tolerated dose (human)    |                    | -0.269    | Numeric (log mg/kg/day) |
| Toxicity hERG I inhibitor               |                    | No        | Categorical (Yes/No)  |
| Toxicity hERG II inhibitor              |                    | Yes       | Categorical (Yes/No)  |
| Toxicity Oral Rat Acute Toxicity (LD50) |                    | 1.919     | Numeric (mol/kg)      |
| Toxicity Oral Rat Chronic Toxicity (LOAEL) |                | 2.112     | Numeric (log mg/kg_bw/day) |
| Toxicity Hepatotoxicity                 |                    | Yes       | Categorical (Yes/No)  |
| Toxicity Skin Sensitisation             |                    | No        | Categorical (Yes/No)  |
| Toxicity T.Pyriformis toxicity          |                    | 0.629     | Numeric (log ug/L)    |
| Toxicity Minnow toxicity                |                    | -1.319    | Numeric (log mM)      |
- For 7-hydroxy-4,8-dimethyl-3-N-(pyridin-4-yl)propanamide coumarin (8)

### Molecule Properties

| Descriptor                     | Value      |
|--------------------------------|------------|
| Molecular Weight              | 338.363 g/mol |
| LogP                          | 3.08174    |
| #Rotatable Bonds              | 4          |
| #Acceptors                    | 5          |
| #Donors                       | 2          |
| Surface Area                  | 143.686    |

### Property Table

| Property                     | Model Name               | Value      | Unit            |
|------------------------------|--------------------------|------------|-----------------|
| Absorption Water solubility |                         | -3.408     | Numeric (log mol/L) |
| Absorption Caco2 permeability|                         | 0.754      | Numeric (log Papp in $10^{-6}$ cm/s) |
| Absorption Intestinal absorption (human) | | 83.921 | Numeric (% Absorbed) |
| Absorption Skin Permeability |                         | -2.897     | Numeric (log Kp) |
| Absorption P-glycoprotein substrate | | Yes | Categorical (Yes/No) |
| Absorption P-glycoprotein I inhibitor | | No | Categorical (Yes/No) |
| Absorption P-glycoprotein II inhibitor | | No | Categorical (Yes/No) |
| Distribution VDss (human)   |                         | 0.134      | Numeric (log L/kg) |
| Distribution Fraction unbound (human) | | 0.075 | Numeric (Fu) |
| Distribution BBB permeability |                         | -0.415     | Numeric (log BB) |
| Distribution CNS permeability |                         | -2.381     | Numeric (log PS) |
| Metabolism CYP2D6 substrate |                         | No         | Categorical (Yes/No) |
| Metabolism CYP3A4 substrate |                         | No         | Categorical (Yes/No) |
| Metabolism CYP1A2 inhibitor |                         | Yes        | Categorical (Yes/No) |
| Metabolism CYP2C19 inhibitor |                         | Yes        | Categorical (Yes/No) |
| Metabolism CYP2C9 inhibitor |                         | Yes        | Categorical (Yes/No) |
| Metabolism CYP2D6 inhibitor |                         | No         | Categorical (Yes/No) |
| Metabolism CYP3A4 inhibitor |                         | No         | Categorical (Yes/No) |
| Excretion Total Clearance    |                         | 0.636      | Numeric (log ml/min/kg) |
| Excretion Renal OCT2 substrate |                     | No         | Categorical (Yes/No) |
| Toxicity AMES toxicity       |                         | No         | Categorical (Yes/No) |
| Toxicity Max. tolerated dose (human) | | 0.067 | Numeric (log mg/kg/day) |
| Toxicity hERG I inhibitor    |                         | No         | Categorical (Yes/No) |
| Toxicity hERG II inhibitor   |                         | No         | Categorical (Yes/No) |
| Toxicity Oral Rat Acute Toxicity (LD50) | | 2.22 | Numeric (mol/kg) |
| Toxicity Oral Rat Chronic Toxicity (LOAEL) | | 1.354 | Numeric (log mg/kg_bw/day) |
| Toxicity Hepatotoxicity      |                         | Yes        | Categorical (Yes/No) |
| Toxicity Skin Sensitisation  |                         | No         | Categorical (Yes/No) |
| Toxicity T.Pyriformis toxicity |                     | 0.622      | Numeric (log ug/L) |
| Toxicity Minnow toxicity     |                         | -0.551     | Numeric (log mM) |
- For 7-hydroxy-4,8-dimethyl-3-N-(1H-imidazol-2-yl)propanamide coumarin (9)

**Molecule Depiction**

![Molecule Depiction](image)

| Descriptor                  | Value          |
|-----------------------------|----------------|
| Molecular Weight            | 327.34 g/mol   |
| LogP                        | 2.40984        |
| #Rotatable Bonds            | 4              |
| #Acceptors                  | 5              |
| #Donors                     | 3              |
| Surface Area                | 136.896        |

**Molecule Properties**

| Property                     | Model Name                  | Value         | Unit                        |
|------------------------------|-----------------------------|---------------|-----------------------------|
| Absorption                   | Water solubility            | -3.133        | Numeric (log mol/L)         |
| Absorption                   | Caco2 permeability          | 0.194         | Numeric (log Papp in 10^-6 cm/s) |
| Absorption                   | Intestinal absorption (human) | 76.284       | Numeric (% Absorbed)        |
| Absorption                   | Skin Permeability           | -2.735        | Numeric (log Kp)            |
| Absorption                   | P-glycoprotein substrate    | Yes           | Categorical (Yes/No)        |
| Absorption                   | P-glycoprotein I inhibitor   | No            | Categorical (Yes/No)        |
| Absorption                   | P-glycoprotein II inhibitor  | No            | Categorical (Yes/No)        |
| Distribution                 | VDss (human)                | -0.108        | Numeric (log L/kg)          |
| Distribution                 | Fraction unbound (human)    | 0.239         | Numeric (Fu)                |
| Distribution                 | BBB permeability            | -1.155        | Numeric (log BB)            |
| Distribution                 | CNS permeability            | -2.736        | Numeric (log PS)            |
| Metabolism                   | CYP2D6 substrate            | No            | Categorical (Yes/No)        |
| Metabolism                   | CYP3A4 substrate            | No            | Categorical (Yes/No)        |
| Metabolism                   | CYP1A2 inhibitor            | Yes           | Categorical (Yes/No)        |
| Metabolism                   | CYP2C19 inhibitor           | No            | Categorical (Yes/No)        |
| Metabolism                   | CYP2C9 inhibitor            | No            | Categorical (Yes/No)        |
| Metabolism                   | CYP2D6 inhibitor            | No            | Categorical (Yes/No)        |
| Metabolism                   | CYP3A4 inhibitor            | No            | Categorical (Yes/No)        |
| Excretion                    | Total Clearance             | 0.839         | Numeric (log ml/min/kg)     |
| Excretion                    | Renal OCT2 substrate        | No            | Categorical (Yes/No)        |
| Toxicity                     | AMES toxicity               | Yes           | Categorical (Yes/No)        |
| Toxicity                     | Max. tolerated dose (human) | 0.541         | Numeric (log mg/kg/day)     |
| Toxicity                     | hERG I inhibitor            | No            | Categorical (Yes/No)        |
| Toxicity                     | hERG II inhibitor           | No            | Categorical (Yes/No)        |
| Toxicity                     | Oral Rat Acute Toxicity (LD50) | 2.045     | Numeric (mol/kg)            |
| Toxicity                     | Oral Rat Chronic Toxicity (LOAEL) | 2.448     | Numeric (log mg/kg_bw/day)  |
| Toxicity                     | Hepatotoxicity              | No            | Categorical (Yes/No)        |
| Toxicity                     | Skin Sensitisation          | No            | Categorical (Yes/No)        |
| Toxicity                     | T. Pyriformis toxicity      | 0.285         | Numeric (log ug/L)          |
| Toxicity                     | Minnow toxicity             | 1.747         | Numeric (log mM)            |
For 7-hydroxy-4,8-dimethyl-3-N-(1H-benzo[d]imidazol-2-yl)propanamide coumarin (10)

| Property                          | Model Name                        | Value   | Unit               |
|-----------------------------------|-----------------------------------|---------|--------------------|
| Absorption Water solubility       | -3.067                            | Numeric (log mol/L) |
| Absorption Caco2 permeability     | 0.404                             | Numeric (log Papp in 10^-6 cm/s) |
| Absorption Intestinal absorption (human) | 84.189                         | Numeric (% Absorbed) |
| Absorption Skin Permeability      | -2.735                            | Numeric (log Kp)      |
| Absorption P-glycoprotein substrate | Yes                             | Categorical (Yes/No) |
| Absorption P-glycoprotein I inhibitor | No                             | Categorical (Yes/No) |
| Absorption P-glycoprotein II inhibitor | Yes                            | Categorical (Yes/No) |
| Distribution VDss (human)         | 0.368                             | Numeric (log L/kg)    |
| Distribution Fraction unbound (human) | 0.082                         | Numeric (Fu)          |
| Distribution BBB permeability     | -1.112                            | Numeric (log BB)      |
| Distribution CNS permeability     | -2.338                            | Numeric (log PS)      |
| Metabolism CYP2D6 substrate       | No                                | Categorical (Yes/No) |
| Metabolism CYP3A4 substrate       | No                                | Categorical (Yes/No) |
| Metabolism CYP1A2 inhibitor       | Yes                               | Categorical (Yes/No) |
| Metabolism CYP2C19 inhibitor      | Yes                               | Categorical (Yes/No) |
| Metabolism CYP2C9 inhibitor       | Yes                               | Categorical (Yes/No) |
| Metabolism CYP2D6 inhibitor       | No                                | Categorical (Yes/No) |
| Metabolism CYP3A4 inhibitor       | Yes                               | Categorical (Yes/No) |
| Excretion Total Clearance         | 1.059                             | Numeric (log ml/min/kg) |
| Excretion Renal OCT2 substrate    | No                                | Categorical (Yes/No) |
| Toxicity AMES toxicity            | Yes                               | Categorical (Yes/No) |
| Toxicity Max. tolerated dose (human) | 0.346                          | Numeric (log mg/kg/day) |
| Toxicity hERG I inhibitor         | No                                | Categorical (Yes/No) |
| Toxicity hERG II inhibitor        | Yes                               | Categorical (Yes/No) |
| Toxicity Oral Rat Acute Toxicity (LD50) | 2.223                          | Numeric (mol/kg)      |
| Toxicity Oral Rat Chronic Toxicity (LOAEL) | 2.921                         | Numeric (log mg/kg_bw/day) |
| Toxicity Hepatotoxicity           | Yes                               | Categorical (Yes/No) |
| Toxicity Skin Sensitisation       | No                                | Categorical (Yes/No) |
| Toxicity T. Pyriformis toxicity   | 0.285                             | Numeric (log ug/L)    |
| Toxicity Minnow toxicity          | -0.646                            | Numeric (log mM)      |
For 7-hydroxy-4,8-dimethyl-3-N-(oxazol-2-yl)propanamide coumarin (11)

| Property                        | Model Name                  | Value      | Unit               |
|---------------------------------|-----------------------------|------------|--------------------|
| **Absorption**                  | Water solubility            | -3.106     | Numeric (log mol/L) |
| **Absorption**                  | Caco2 permeability          | 0.606      | Numeric (log Papp in $10^{-6}$ cm/s) |
| **Absorption**                  | Intestinal absorption (human)| 85.899     | Numeric (% Absorbed) |
| **Absorption**                  | Skin Permeability           | -2.901     | Numeric (log Kp)    |
| **Absorption**                  | P-glycoprotein substrate    | Yes        | Categorical (Yes/No) |
| **Absorption**                  | P-glycoprotein I inhibitor  | No         | Categorical (Yes/No) |
| **Absorption**                  | P-glycoprotein II inhibitor | No         | Categorical (Yes/No) |
| **Distribution**                | VDss (human)                | 0.081      | Numeric (log L/kg)  |
| **Distribution**                | Fraction unbound (human)    | 0.084      | Numeric (Fu)        |
| **Distribution**                | BBB permeability            | -0.575     | Numeric (log BB)    |
| **Distribution**                | CNS permeability            | -2.548     | Numeric (log PS)    |
| **Metabolism**                  | CYP2D6 substrate            | No         | Categorical (Yes/No) |
| **Metabolism**                  | CYP3A4 substrate            | No         | Categorical (Yes/No) |
| **Metabolism**                  | CYP1A2 inhibitor            | Yes        | Categorical (Yes/No) |
| **Metabolism**                  | CYP2C19 inhibitor           | Yes        | Categorical (Yes/No) |
| **Metabolism**                  | CYP2C9 inhibitor            | No         | Categorical (Yes/No) |
| **Metabolism**                  | CYP2D6 inhibitor            | No         | Categorical (Yes/No) |
| **Metabolism**                  | CYP3A4 inhibitor            | No         | Categorical (Yes/No) |
| **Excretion**                   | Total Clearance             | 0.729      | Numeric (log ml/min/kg) |
| **Excretion**                   | Renal OCT2 substrate        | No         | Categorical (Yes/No) |
| **Toxicity**                    | Ames toxicity               | No         | Categorical (Yes/No) |
| **Toxicity**                    | Max. tolerated dose (human) | 0.159      | Numeric (log mg/kg/day) |
| **Toxicity**                    | hERG I inhibitor            | No         | Categorical (Yes/No) |
| **Toxicity**                    | hERG II inhibitor           | No         | Categorical (Yes/No) |
| **Toxicity**                    | Oral Rat acute Toxicity (LD50) | 2.07   | Numeric (mol/kg) |
| **Toxicity**                    | Oral Rat Chronic Toxicity (LOAEL) | 1.565 | Numeric (log mg/kg_bw/day) |
| **Toxicity**                    | Hepatotoxicity              | Yes        | Categorical (Yes/No) |
| **Toxicity**                    | Skin Sensitisation          | No         | Categorical (Yes/No) |
| **Toxicity**                    | T.Pyrophormis toxicity      | 0.624      | Numeric (log ug/L)  |
| **Toxicity**                    | Minnow toxicity             | -0.411     | Numeric (log mM)    |
### Molecule Depiction
![Molecule Depiction Image]

### Molecule Properties

| Descriptor                      | Value         |
|---------------------------------|---------------|
| Molecular Weight                | 378.384 g/mol |
| LogP                            | 3.82794       |
| #Rotatable Bonds                | 4             |
| #Acceptors                      | 6             |
| #Donors                         | 2             |
| Surface Area                    | 159.162       |

| Property                        | Model Name         | Value         | Unit                |
|---------------------------------|--------------------|---------------|---------------------|
| Absorption                      | Water solubility   | -4.27         | Numeric (log mol/L) |
| Absorption                      | Caco2 permeability | 0.337         | Numeric (log Papp in 10^-6 cm/s) |
| Absorption                      | Intestinal absorption (human) | 93.803 | Numeric (% Absorbed) |
| Absorption                      | Skin Permeability  | -2.74         | Numeric (log Kp)    |
| Absorption                      | P-glycoprotein substrate | Yes | Categorical (Yes/No) |
| Absorption                      | P-glycoprotein I inhibitor | Yes | Categorical (Yes/No) |
| Absorption                      | P-glycoprotein II inhibitor | Yes | Categorical (Yes/No) |
| Distribution                    | VDss (human)       | -0.413        | Numeric (log L/kg)  |
| Distribution                    | Fraction unbound (human) | 0.01 | Numeric (Fu) |
| Distribution                    | BBB permeability   | -0.337        | Numeric (log BB)    |
| Distribution                    | CNS permeability   | -2.193        | Numeric (log PS)    |
| Metabolism                      | CYP2D6 substrate  | No            | Categorical (Yes/No) |
| Metabolism                      | CYP3A4 substrate  | Yes           | Categorical (Yes/No) |
| Metabolism                      | CYP1A2 inhibitor   | Yes           | Categorical (Yes/No) |
| Metabolism                      | CYP2C19 inhibitor  | Yes           | Categorical (Yes/No) |
| Metabolism                      | CYP2C9 inhibitor   | Yes           | Categorical (Yes/No) |
| Metabolism                      | CYP2D6 inhibitor   | No            | Categorical (Yes/No) |
| Metabolism                      | CYP3A4 inhibitor   | Yes           | Categorical (Yes/No) |
| Excretion                       | Total Clearance    | 0.617         | Numeric (log ml/min/kg) |
| Excretion                       | Renal OCT2 substrate | No | Categorical (Yes/No) |
| Toxicity                        | AMES toxicity      | No            | Categorical (Yes/No) |
| Toxicity                        | Max. tolerated dose (human) | 0.155 | Numeric (log mg/kg/day) |
| Toxicity                        | hERG I inhibitor   | No            | Categorical (Yes/No) |
| Toxicity                        | hERG II inhibitor  | Yes           | Categorical (Yes/No) |
| Toxicity                        | Oral Rat Acute Toxicity (LD50) | 2.197 | Numeric (mol/kg) |
| Toxicity                        | Oral Rat Chronic Toxicity (LOAEL) | 2.066 | Numeric (log mg/kg_bw/day) |
| Toxicity                        | Hepatotoxicity     | Yes           | Categorical (Yes/No) |
| Toxicity                        | Skin Sensitisation | No            | Categorical (Yes/No) |
| Toxicity                        | T. Pyriformis toxicity | 0.319 | Numeric (log ug/L) |
| Toxicity                        | Minnow toxicity    | -2.39         | Numeric (log mM)    |
For 7-hydroxy-4,8-dimethyl-3-N-(1H-indol-5-y1)propanamide coumarin (13)

| Property                  | Model Name                  | Value       | Unit                      |
|---------------------------|-----------------------------|-------------|---------------------------|
| **Molecule Properties**   |                             |             |                           |
| Molecular Weight          |                             | 376.412 g/mol |                           |
| LogP                      |                             | 4.16804     |                           |
| #Rotatable Bonds          |                             | 4           |                           |
| #Acceptors                |                             | 4           |                           |
| #Donors                   |                             | 3           |                           |
| Surface Area              |                             | 160.358     |                           |
| **Property**              | **Model Name**              | **Value**   | **Unit**                  |
| Absorption Water solubility| Water solubility            | -4.156      | Numeric (log mol/L)       |
| Absorption Caco2 permeability|                             | 0.403       | Numeric (log Papp in 10^-6 cm/s) |
| Absorption Intestinal absorption (human) | Intestinal absorption (human) | 89.923      | Numeric (% Absorbed)      |
| Absorption Skin Permeability | Skin Permeability           | -2.745      | Numeric (log Kp)          |
| Absorption P-glycoprotein substrate | P-glycoprotein substrate | Yes         | Categorical (Yes/No)     |
| Absorption P-glycoprotein I inhibitor | P-glycoprotein I inhibitor | Yes         | Categorical (Yes/No)     |
| Absorption P-glycoprotein II inhibitor | P-glycoprotein II inhibitor | Yes         | Categorical (Yes/No)     |
| Distribution VDss (human)  | VDss (human)                | -0.238      | Numeric (log L/kg)        |
| Distribution Fraction unbound (human) | Fraction unbound (human) | 0           | Numeric (Fu)              |
| Distribution BBB permeability |                             | -0.792      | Numeric (log BB)          |
| Distribution CNS permeability |                             | -1.997      | Numeric (log PS)          |
| Metabolism CYP2D6 substrate | CYP2D6 substrate            | No          | Categorical (Yes/No)     |
| Metabolism CYP3A4 substrate | CYP3A4 substrate            | Yes         | Categorical (Yes/No)     |
| Metabolism CYP1A2 inhibitor | CYP1A2 inhibitor            | Yes         | Categorical (Yes/No)     |
| Metabolism CYP2C9 inhibitor | CYP2C9 inhibitor            | Yes         | Categorical (Yes/No)     |
| Metabolism CYP2D6 inhibitor | CYP2D6 inhibitor            | No          | Categorical (Yes/No)     |
| Metabolism CYP3A4 inhibitor | CYP3A4 inhibitor            | Yes         | Categorical (Yes/No)     |
| Excretion Total Clearance  | Total Clearance             | 0.595       | Numeric (log ml/min/kg)   |
| Excretion Renal OCT2 substrate | Renal OCT2 substrate       | No          | Categorical (Yes/No)     |
| Toxicity AMES toxicity     | AMES toxicity               | Yes         | Categorical (Yes/No)     |
| Toxicity Max. tolerated dose (human) | Max. tolerated dose (human) | -0.12       | Numeric (log mg/kg/day)   |
| Toxicity hERG I inhibitor  | hERG I inhibitor            | No          | Categorical (Yes/No)     |
| Toxicity hERG II inhibitor | hERG II inhibitor           | Yes         | Categorical (Yes/No)     |
| Toxicity Oral Rat Acute Toxicity (LD50) | Oral Rat Acute Toxicity (LD50) | 2.468       | Numeric (mol/kg)          |
| Toxicity Oral Rat Chronic Toxicity (LOAEL) | Oral Rat Chronic Toxicity (LOAEL) | 2.353       | Numeric (log mg/kg_bw/day) |
| Toxicity Hepatotoxicity    | Hepatotoxicity              | Yes         | Categorical (Yes/No)     |
| Toxicity Skin Sensitisation | Skin Sensitisation          | No          | Categorical (Yes/No)     |
| Toxicity T. Pyriformis toxicity | T. Pyriformis toxicity     | 0.328       | Numeric (log ug/L)        |
| Toxicity Minnow toxicity   | Minnow toxicity             | -1.317      | Numeric (log mM)          |
- For 7-hydroxy-4,8-dimethyl-3-N-(6-oxo-6,9-dihydro-1H-purin-2-yl)propanamide coumarin (14)

![Molecule Depiction](image)

| Molecule Properties | Descriptor | Value          |
|---------------------|------------|----------------|
|                     | Molecular Weight | 395.375 g/mol |
|                     | LogP         | 1.64634        |
|                     | #Rotatable Bonds | 4              |
|                     | #Acceptors   | 7              |
|                     | #Donors      | 4              |
|                     | Surface Area | 162.178        |

| Property               | Model Name                     | Value          | Unit               |
|------------------------|--------------------------------|----------------|--------------------|
| Absorption             | Water solubility               | -2.954         | Numeric (log mol/L) |
| Absorption             | Caco2 permeability             | -0.593         | Numeric (log Papp in 10^-6 cm/s) |
| Absorption             | Intestinal absorption (human)  | 60.724         | Numeric (% Absorbed) |
| Absorption             | Skin Permeability              | -2.735         | Numeric (log Kp)    |
| Absorption             | P-glycoprotein substrate       | Yes            | Categorical (Yes/No) |
| Absorption             | P-glycoprotein I inhibitor     | No             | Categorical (Yes/No) |
| Absorption             | P-glycoprotein II inhibitor    | No             | Categorical (Yes/No) |
| Distribution           | VDss (human)                   | -0.134         | Numeric (log L/kg)  |
| Distribution           | Fraction unbound (human)       | 0.301          | Numeric (Fu)        |
| Distribution           | BBB permeability               | -1.803         | Numeric (log BB)    |
| Distribution           | CNS permeability               | -4.07          | Numeric (log PS)    |
| Metabolism             | CYP2D6 substrate               | No             | Categorical (Yes/No) |
| Metabolism             | CYP3A4 substrate               | No             | Categorical (Yes/No) |
| Metabolism             | CYP1A2 inhibitor               | No             | Categorical (Yes/No) |
| Metabolism             | CYP2C19 inhibitor              | No             | Categorical (Yes/No) |
| Metabolism             | CYP2C9 inhibitor               | No             | Categorical (Yes/No) |
| Metabolism             | CYP2D6 inhibitor               | No             | Categorical (Yes/No) |
| Metabolism             | CYP3A4 inhibitor               | No             | Categorical (Yes/No) |
| Excretion              | Total Clearance                | 0.742          | Numeric (log ml/min/kg) |
| Excretion              | Renal OCT2 substrate           | No             | Categorical (Yes/No) |
| Toxicity               | Ames toxicity                  | No             | Categorical (Yes/No) |
| Toxicity               | Max. tolerated dose (human)    | 0.465          | Numeric (log mg/kg/day) |
| Toxicity               | hERG I inhibitor               | No             | Categorical (Yes/No) |
| Toxicity               | hERG II inhibitor              | Yes            | Categorical (Yes/No) |
| Toxicity               | Oral Rat Acute Toxicity (LD50) | 2.391          | Numeric (mol/kg)    |
| Toxicity               | Oral Rat Chronic Toxicity (LOAEL) | 3.473         | Numeric (log mg/kg_bw/day) |
| Toxicity               | Hepatotoxicity                 | No             | Categorical (Yes/No) |
| Toxicity               | Skin Sensitisation             | No             | Categorical (Yes/No) |
| Toxicity               | T. Pyriformis toxicity         | 0.285          | Numeric (log ug/L)  |
| Toxicity               | Minnow toxicity                | 1.72           | Numeric (log mM)    |
For 7-hydroxy-4,8-dimethyl-3-N-(2-oxo-1,2-dihydropyrimidin-4-yl)propanamide coumarin (15)

| Property                        | Model Name                  | Value       | Unit                     |
|---------------------------------|-----------------------------|-------------|--------------------------|
| **Absorption**                  | Water solubility            | -2.952      | Numeric (log mol/L)      |
|                                 | Caco2 permeability          | -0.124      | Numeric (log Papp in 10^6 cm/s) |
|                                 | Intestinal absorption (human) | 67.793      | Numeric (% Absorbed)     |
|                                 | Skin Permeability           | -2.763      | Numeric (log Kp)         |
| **Absorption**                  | P-glycoprotein substrate    | Yes         | Categorical (Yes/No)     |
|                                 | P-glycoprotein I inhibitor  | No          | Categorical (Yes/No)     |
|                                 | P-glycoprotein II inhibitor | No          | Categorical (Yes/No)     |
| **Distribution**                | VDss (human)                | 0.372       | Numeric (log L/kg)       |
|                                 | Fraction unbound (human)    | 0.076       | Numeric (Fu)             |
|                                 | BBB permeability            | -1.167      | Numeric (log BB)         |
| **Distribution**                | CNS permeability            | -2.893      | Numeric (log PS)         |
| **Metabolism**                  | CYP2D6 substrate            | No          | Categorical (Yes/No)     |
|                                 | CYP3A4 substrate            | No          | Categorical (Yes/No)     |
|                                 | CYP1A2 inhibitor            | No          | Categorical (Yes/No)     |
|                                 | CYP2C19 inhibitor           | No          | Categorical (Yes/No)     |
|                                 | CYP2C9 inhibitor            | No          | Categorical (Yes/No)     |
|                                 | CYP2D6 inhibitor            | No          | Categorical (Yes/No)     |
|                                 | CYP3A4 inhibitor            | No          | Categorical (Yes/No)     |
| **Excretion**                   | Total Clearance             | 0.75        | Numeric (log ml/min/kg)  |
| **Toxicity**                    | AMES toxicity               | No          | Categorical (Yes/No)     |
|                                 | Max. tolerated dose (human) | 0.653       | Numeric (log mg/kg/day)  |
|                                 | hERG I inhibitor            | No          | Categorical (Yes/No)     |
|                                 | hERG II inhibitor           | No          | Categorical (Yes/No)     |
|                                 | Oral Rat Acute Toxicity (LD50) | 2.173   | Numeric (mol/kg)       |
|                                 | Oral Rat Chronic Toxicity (LOAEL) | 1.896 | Numeric (log mg/kg_bw/day) |
| **Toxicity**                    | Hepatotoxicity              | Yes         | Categorical (Yes/No)     |
|                                 | Skin Sensitisation          | No          | Categorical (Yes/No)     |
| **Toxicity**                    | T. Pyriformis toxicity      | 0.321       | Numeric (log ug/L)       |
|                                 | Minnow toxicity             | 1.2         | Numeric (log mM)         |

**Molecule Depiction**

**Molecule Properties**

- **Descriptor**
  - **Value**
    - **Molecular Weight**: 355.35 g/mol
    - **LogP**: 1.77004
    - **#Rotatable Bonds**: 4
    - **#Acceptors**: 6
    - **#Donors**: 3
    - **Surface Area**: 147.068
For 7-hydroxy-4,8-dimethyl-3-N-(4,9-dihydro-3H-purin-6-yl)propanamide coumarin (16)

**Molecule Properties**

| Descriptor             | Value          |
|------------------------|----------------|
| Molecular Weight       | 381.392 g/mol  |
| LogP                   | 0.93084        |
| #Rotatable Bonds       | 3              |
| #Acceptors             | 8              |
| #Donors                | 3              |
| Surface Area           | 159.459        |

**Property**  | **Model Name** | **Value** | **Unit** |
|---------------|----------------|-----------|----------|
| Absorption    | Water solubility | -3.026    | Numeric (log mol/L) |
| Absorption    | Caco2 permeability | -0.04    | Numeric (log Papp in 10^-6 cm/s) |
| Absorption    | Intestinal absorption (human) | 74.646 | Numeric (% Absorbed) |
| Absorption    | Skin Permeability | -3.238 | Numeric (log Kp) |
| Absorption    | P-glycoprotein substrate | Yes | Categorical (Yes/No) |
| Absorption    | P-glycoprotein I inhibitor | Yes | Categorical (Yes/No) |
| Absorption    | P-glycoprotein II inhibitor | No | Categorical (Yes/No) |
| Distribution  | VDss (human) | 0.272 | Numeric (log L/kg) |
| Distribution  | Fraction unbound (human) | 0.256 | Numeric (Fu) |
| Distribution  | BBB permeability | -0.644 | Numeric (log BB) |
| Distribution  | CNS permeability | -2.803 | Numeric (log PS) |
| Metabolism    | CYP2D6 substrate | No | Categorical (Yes/No) |
| Metabolism    | CYP3A4 substrate | No | Categorical (Yes/No) |
| Metabolism    | CYP1A2 inhibitor | No | Categorical (Yes/No) |
| Metabolism    | CYP2C19 inhibitor | No | Categorical (Yes/No) |
| Metabolism    | CYP2C9 inhibitor | No | Categorical (Yes/No) |
| Metabolism    | CYP2D6 inhibitor | No | Categorical (Yes/No) |
| Metabolism    | CYP3A4 inhibitor | No | Categorical (Yes/No) |
| Excretion     | Total Clearance | 0.886 | Numeric (log ml/min/kg) |
| Excretion     | Renal OCT2 substrate | No | Categorical (Yes/No) |
| Toxicity      | AMES toxicity | No | Categorical (Yes/No) |
| Toxicity      | Max. tolerated dose (human) | -0.525 | Numeric (log mg/kg/day) |
| Toxicity      | hERG I inhibitor | No | Categorical (Yes/No) |
| Toxicity      | hERG II inhibitor | Yes | Categorical (Yes/No) |
| Toxicity      | Oral Rat Acute Toxicity (LD50) | 1.947 | Numeric (mol/kg) |
| Toxicity      | Oral Rat Chronic Toxicity (LOAEL) | 1.997 | Numeric (log mg/kg_bw/day) |
| Toxicity      | Hepatotoxicity | Yes | Categorical (Yes/No) |
| Toxicity      | Skin Sensitisation | No | Categorical (Yes/No) |
| Toxicity      | T.Pyrrformis toxicity | 0.513 | Numeric (log ug/L) |
| Toxicity      | Minnow toxicity | 2.287 | Numeric (log mM) |
For 7-hydroxy-4,8-dimethyl-3-N-(benzo[d]thiazol-2-yl)propenamide coumarin (17)

### Molecule Depiction
![Molecule Depiction](image)

### Molecule Properties
| Descriptor                  | Value          |
|-----------------------------|----------------|
| Molecular Weight            | 394.452 g/mol  |
| LogP                        | 4.29644        |
| #Rotatable Bonds            | 4              |
| #Acceptors                  | 6              |
| #Donors                     | 2              |
| Surface Area                | 164.009        |

### Property Model Name Value Unit

| Property                  | Model Name          | Value       | Unit                |
|---------------------------|---------------------|-------------|--------------------|
| Absorption                | Water solubility    | -4.424      | Numeric (log mol/L) |
| Absorption                | Caco2 permeability  | 0.405       | Numeric (log Papp in 10^-6 cm/s) |
| Absorption                | Intestinal absorption (human) | 95.086 | Numeric (% Absorbed) |
| Absorption                | Skin Permeability   | -2.74       | Numeric (log Kp)    |
| Absorption                | P-glycoprotein substrate | Yes      | Categorical (Yes/No) |
| Absorption                | P-glycoprotein I inhibitor | Yes    | Categorical (Yes/No) |
| Absorption                | P-glycoprotein II inhibitor | Yes   | Categorical (Yes/No) |
| Distribution              | VDss (human)        | -0.354      | Numeric (log L/kg)  |
| Distribution              | Fraction unbound (human) | 0.011 | Numeric (Fu)       |
| Distribution              | BBB permeability    | -0.334      | Numeric (log BB)    |
| Distribution              | CNS permeability    | -2.083      | Numeric (log PS)    |
| Metabolism                | CYP2D6 substrate    | No          | Categorical (Yes/No) |
| Metabolism                | CYP3A4 substrate    | Yes         | Categorical (Yes/No) |
| Metabolism                | CYP1A2 inhibitor    | Yes         | Categorical (Yes/No) |
| Metabolism                | CYP2C19 inhibitor   | Yes         | Categorical (Yes/No) |
| Metabolism                | CYP2C9 inhibitor    | Yes         | Categorical (Yes/No) |
| Metabolism                | CYP2D6 inhibitor    | No          | Categorical (Yes/No) |
| Metabolism                | CYP3A4 inhibitor    | Yes         | Categorical (Yes/No) |
| Excretion                 | Total Clearance     | -0.23       | Numeric (log ml/min/kg) |
| Excretion                 | Renal OCT2 substrate | No      | Categorical (Yes/No) |
| Toxicity                  | AMES toxicity       | No          | Categorical (Yes/No) |
| Toxicity                  | Max. tolerated dose (human) | 0.182 | Numeric (log mg/kg/day) |
| Toxicity                  | hERG I inhibitor    | No          | Categorical (Yes/No) |
| Toxicity                  | hERG II inhibitor   | Yes         | Categorical (Yes/No) |
| Toxicity                  | Oral Rat Acute Toxicity (LD50) | 2.213 | Numeric (mol/kg) |
| Toxicity                  | Oral Rat Chronic Toxicity (LOAEL) | 2.003 | Numeric (log mg/kg bw/day) |
| Toxicity                  | Hepatotoxicity      | Yes         | Categorical (Yes/No) |
| Toxicity                  | Skin Sensitisation  | No          | Categorical (Yes/No) |
| Toxicity                  | T.Pyrimidales toxicity | 0.32    | Numeric (log ug/L)  |
| Toxicity                  | Minnow toxicity     | -2.668      | Numeric (log mM)    |
For 4,7-dihydroxy-3-(3-oxo-1-phenylbutyl)-coumarin (Warfarin or Coumadin)

![Molecule Depiction](image)

| Molecule Properties | Descriptor          | Value       |
|---------------------|---------------------|-------------|
| Molecular Weight    | 308.333 g/mol       |
| LogP                | 3.6096              |
| #Rotatable Bonds    | 4                   |
| #Acceptors          | 4                   |
| #Donors             | 1                   |
| Surface Area        | 132.552             |

| Property            | Model Name                  | Value       | Unit               |
|---------------------|-----------------------------|-------------|--------------------|
| Absorption          | Water solubility            | -4.296      | Numeric (log mol/L) |
| Absorption          | Caco2 permeability          | 0.955       | Numeric (log Papp in 10^-6 cm/s) |
| Absorption          | Intestinal absorption (human) | 96.137      | Numeric (% Absorbed) |
| Absorption          | Skin Permeability           | -2.787      | Numeric (log Kp)    |
| Absorption          | P-glycoprotein substrate    | No          | Categorical (Yes/No) |
| Absorption          | P-glycoprotein I inhibitor  | No          | Categorical (Yes/No) |
| Absorption          | P-glycoprotein II inhibitor | Yes         | Categorical (Yes/No) |
| Distribution        | VDss (human)                | -0.137      | Numeric (log L/kg)  |
| Distribution        | Fraction unbound (human)    | 0.075       | Numeric (Fu)       |
| Distribution        | BBB permeability            | -0.14       | Numeric (log BB)    |
| Distribution        | CNS permeability            | -2.059      | Numeric (log PS)    |
| Metabolism          | CYP2D6 substrate            | No          | Categorical (Yes/No) |
| Metabolism          | CYP3A4 substrate            | Yes         | Categorical (Yes/No) |
| Metabolism          | CYP1A2 inhibitor            | Yes         | Categorical (Yes/No) |
| Metabolism          | CYP2C19 inhibitor           | Yes         | Categorical (Yes/No) |
| Metabolism          | CYP2C9 inhibitor            | Yes         | Categorical (Yes/No) |
| Metabolism          | CYP2D6 inhibitor            | No          | Categorical (Yes/No) |
| Metabolism          | CYP3A4 inhibitor            | Yes         | Categorical (Yes/No) |
| Excretion           | Total Clearance             | 0.803       | Numeric (log ml/min/kg) |
| Excretion           | Renal OCT2 substrate        | No          | Categorical (Yes/No) |
| Toxicity            | AMES toxicity               | No          | Categorical (Yes/No) |
| Toxicity            | Max. tolerated dose (human) | 0.289       | Numeric (log mg/kg/day) |
| Toxicity            | hERG I inhibitor            | No          | Categorical (Yes/No) |
| Toxicity            | hERG II inhibitor           | Yes         | Categorical (Yes/No) |
| Toxicity            | Oral Rat Acute Toxicity (LD50) | 2.568     | Numeric (mol/kg) |
| Toxicity            | Oral Rat Chronic Toxicity (LOAEL) | 1.593   | Numeric (log mg/kg_bw/day) |
| Toxicity            | Hepatotoxicity              | Yes         | Categorical (Yes/No) |
| Toxicity            | Skin Sensitisation          | No          | Categorical (Yes/No) |
| Toxicity            | T.Pyriformis toxicity       | 0.573       | Numeric (log ug/L)  |
| Toxicity            | Minnow toxicity             | -0.029      | Numeric (log mM)    |