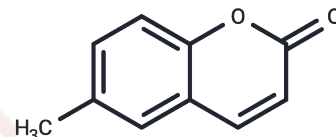


## 6-Methylcoumarin

## Chemical Properties

|                   |   |
|-------------------|---|
| CAS No. :         | 92-48-8   |
| Formula:          | C <sub>10</sub> H <sub>8</sub> O <sub>2</sub>   |
| Molecular Weight: | 160.17  |
| Storage:          | Powder: -20°C for 3 years   In solvent: -80°C for 1 year<br>Actual storage temperature shall be subject to the COA. |



## Biological Description

|               |  |
|---------------|--|
| Description   | 6-Methylcoumarin (Toncarine) (6MC) is a semisynthetic coumarin with important in vitro and in vivo anti-inflammatory activity.   |
| Targets(IC50) | Others   |
| In vitro      | Transport experiments with Caco-2 cells showed that 6MC presented high permeability at all concentrations evaluated. suggested that 6MC could be transported across the gut wall by passive diffusion  |
| In vivo       | 6-Methylcoumarin(6MC) could be transported across the gut wall by passive diffusion. The maximum concentration (C <sub>max</sub> ) was 17.13 ± 2.90 µg/mL at maximum time (T <sub>max</sub> ) of 30 min for the oral route and C <sub>max</sub> 26.18 ± 2.47 µg/mL at 6.0 min for the intraperitoneal administration, with elimination constant of (K <sub>e</sub> ) 0.0070 min <sup>-1</sup> and a short life half time of (T <sub>1/2</sub> ) lower that 120 min. 6MC has high accumulation in the liver, and widespread distribution in all the organs evaluated.   |
| Cell Research | The determination of in vitro intestinal permeability of 6MC was carried out under sink conditions in a series of pH-gradient bidirectional transport experiments with Caco-2 cells. Before the experiments, cell monolayers were rinsed with Hank's balanced salt solution (HBSS) and equilibrated for 30 min at 37 °C. The integrity of the monolayers was assessed before and after the experiments, by transepithelial electrical resistance (TEER) measurement. Only monolayers with TEER values above 200 Ωcm <sup>2</sup> were considered. A stock solution of 6MC (10 mM DMSO) was diluted to final concentration of 10, 25, 50 or 100 µM in HBSS pH 6.5 (apical transport buffer) or pH 7.4 (basolateral transport buffer). Bidirectional experiments (apical-to-basolateral [AB] and basolateral-to-apical [BA]) were initiated by adding 6MC solutions to the donor compartment, and fresh buffer to the acceptor compartment. Caco-2 cell monolayers were incubated for 1 h at 37 °C under constant stirring (150 rpm). Receiver compartments were sampled at 0, 15, 30, 45 and 60 min, refilled with an equivalent amount of transport buffer, and samples were submitted to analysis by HPLC/UV. |

## Solubility Information

|            |  |
|------------|--|
| Solubility | DMSO: 55 mg/mL (343.39 mM),Sonication is recommended.<br>(< 1 mg/ml refers to the product slightly soluble or insoluble) |
|------------|--|

## A DRUG SCREENING EXPERT

|                     |   |
|---------------------|---|
| In vivo Formulation | 10% DMSO+40% PEG300+5% Tween 80+45% Saline: 2 mg/mL (12.49 mM),Sonication is recommended.<br><i>Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.</i> |
|---------------------|---|

### Preparing Stock Solutions

|       | 1mg       | 5mg        | 10mg       |
|-------|-----------|------------|------------|
| 1 mM  | 6.2434 mL | 31.2168 mL | 62.4337 mL |
| 5 mM  | 1.2487 mL | 6.2434 mL  | 12.4867 mL |
| 10 mM | 0.6243 mL | 3.1217 mL  | 6.2434 mL  |
| 50 mM | 0.1249 mL | 0.6243 mL  | 1.2487 mL  |

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

### Reference

Cárdenas Paola Andrea, Kratz Jadel Müller, Hernández Aura, et al. In vitro intestinal permeability studies, pharmacokinetics and tissue distribution of 6-methylcoumarin after oral and intraperitoneal administration in Wistar rats[J]. Brazilian Journal of Pharmaceutical Sciences, 2017, 53(1).

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