

Product Data Sheet

Product Name: PDM 2
Cat. No.: GC11817

Chemical Properties

Cas. No. 688348-25-6

Chemical Name 1,3-dichloro-5-[(1E)-2-(4-chlorophenyl)ethenyl]-benzene

SMILES Clc1ccc(cc1)\C=C/c1cc(Cl)cc(Cl)c1

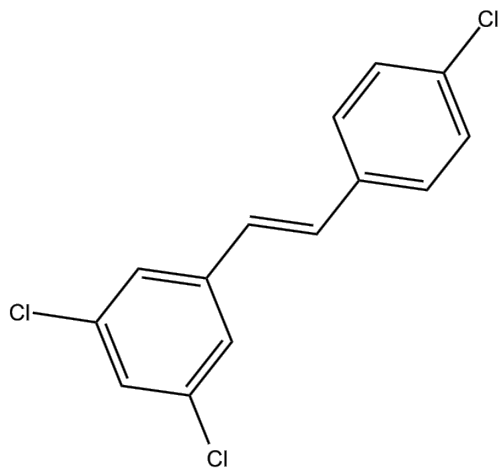
Formula $C_{14}H_9Cl_3$ M.Wt 283.6

Solubility $\leq 2\text{mg/ml}$ in ethanol; 30mg/ml in DMSO; 30mg/ml in dimethyl formamide
Storage Store at -20°C

General tips For obtaining a higher solubility, please warm the tube at 37°C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution: ship with blue ice. All other available size: ship with RT, or blue ice upon request.

Structure



Background

Caution: Product has not been fully validated for medical applications. For research use only.

Tel: (909) 407-4943 Fax: (626) 353-8530 E-mail: tech@glpbio.com

Address: 10292 Central Ave. #205, Montclair, CA, USA

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$K_i = 1.2 \text{ nM}$

PDM 2 is a potent and selective aryl hydrocarbon receptor (AhR) antagonist.

The aryl hydrocarbon receptor (AhR) is a ligand-dependent intracellular transcription factor whose ligands include some of the most infamous xenobiotics, such as dioxin, benzo[a]pyrene, and various polyaromatics from soot and coal tar.

In vitro: In a previous screening study, it was found that the replacement of resveratrol hydroxyls by the same substituent produced compounds with the following order of affinity: OH (resveratrol) , OMe < F < CF₃ < Cl (PDM 2). PDM 2 exhibited a K_i of 1.25 for AhR and no affinity for ER, indicating that replacement of hydroxyl with chloride could abolish binding on ER and dramatically increase the affinity for AhR. Moreover, among its analogs PDM 2 was the most potent AhR antagonists in this series, being 10-fold more efficient than resveratrol. PDM 2, devoid of measurable affinity for ER, did not display any effect on ER-driven transcription. Therefore, PDM 2 was considered as a selective AhR modulator with regard to ER. In addition, its trimethoxylated derivatives and 3,5-methoxy derivatives were able to induce cytotoxicity at doses lower than 100 nM, which was consistent with previous data. 3,5-Methoxy derivatives, however, only showed cytotoxicity at concentrations higher than 10 μM [1].

In vivo: Up to now, there is no animal in vivo data reported.

Clinical trial: So far, no clinical study has been conducted.

Reference:

[1] de Medina, P. ,Casper, R.,Savouret, J.F., et al. Synthesis and biological properties of new stilbene derivatives of resveratrol as new selective aryl hydrocarbon modulators. Journal of Medicinal Chemistry 48, 287-291 (2005).

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