

**Product Name:** AGI 5198

**Catalog No.:** 7087

**Batch No.:** 2

CAS Number: 1355326-35-0

IUPAC Name: *N*-[2-(Cyclohexylamino)-1-(2-methylphenyl)-2-oxoethyl]-*N*-(3-fluorophenyl)-2-methyl-1*H*-imidazole-1-acetamide

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>27</sub>H<sub>31</sub>FN<sub>4</sub>O<sub>2</sub>·¼H<sub>2</sub>O

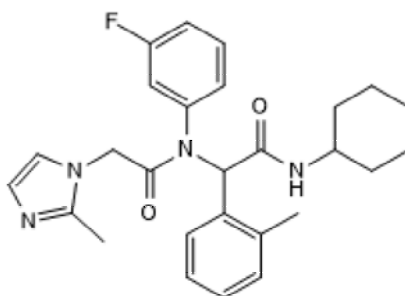
**Batch Molecular Weight:** 467.06

**Physical Appearance:** White solid

**Solubility:** DMSO to 50 mM  
ethanol to 10 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**HPLC:** Shows 99.6% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	69.43	6.8	12
Found	69.56	6.8	11.96

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**Description:**

Potent and selective inhibitor of mutant isocitrate dehydrogenase 1 (mIDH1; IC<sub>50</sub> = 70 nM). Selective for mIDH1 over wild-type IDH1 and IDH2. Inhibits production of oncometabolite D-2 hydroxyglutarate. Attenuates growth of glioma cells containing mIDH1, but not wild-type IDH1, in vitro and in vivo. Also inhibits growth of fibrosarcoma and chondrosarcoma cells bearing mIDH1.

**Physical and Chemical Properties:**

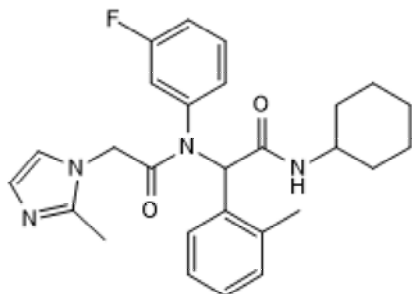
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Batch Molecular Weight: 467.06

Physical Appearance: White solid

**Minimum Purity:** ≥98%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

**Solubility & Usage Info:**

DMSO to 50 mM

ethanol to 10 mM

**Stability and Solubility Advice:**

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

**SOLIDS:** Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

**SOLUTIONS:** We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

**References:**

**Badur et al** (2018) Oncogenic R132 IDH1 mutations limit NADPH for *de novo* lipogenesis through (D)2-hydroxyglutarate production in fibrosarcoma cells. *Cell Rep.* **25** 1018. PMID: 30355481.

**Li et al** (2015) Treatment with a small molecule mutant IDH1 inhibitor suppresses tumorigenic activity and decreases production of the oncometabolite 2-hydroxyglutarate in human chondrosarcoma cells. *PLoS ONE* **10** e0133813. PMID: 26368816.

**Rohle et al** (2013) An inhibitor of mutant IDH1 delays growth and promotes differentiation of glioma cells. *Science* **340** 626. PMID: 23558169.

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