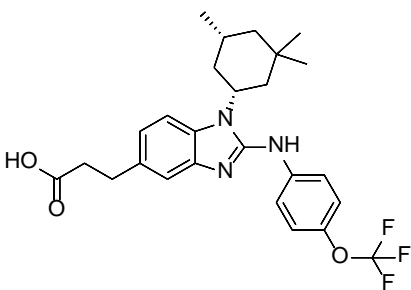


# Product data sheet



MedKoo Cat#: 206773 Name: BAY-1436032 CAS#: 1803274-65-8 Chemical Formula: C <sub>26</sub> H <sub>30</sub> F <sub>3</sub> N <sub>3</sub> O <sub>3</sub> Exact Mass: 489.2239 Molecular Weight: 489.54	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years. In solvent: -80°C 3 months; -20°C 2 weeks.

## 1. Product description:

BAY-1436032 is a potent, selective and orally available inhibitor of mutant Isocitrate Dehydrogenase 1 (mIDH1). BAY 1436032 is a double-digit nanomolar and selective pan-inhibitor of the enzymatic activity of various IDH1-R132X mutants in vitro and displayed potent inhibition of 2-HG release (nanomolar range) in patient derived and engineered cell lines expressing different IDH1 mutants. In line with the proposed mode of action, a concentration-dependent lowering of 2-HG was observed in vitro accompanied by differentiation and maturation of mIDH1 tumor cells. Furthermore, BAY 1436032 showed a favourable selectivity profile against wtIDH1/2 and a large panel of off-targets in vitro.

## 2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under “QC And Documents” section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

## 3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	111.50	227.76
Ethanol	98.0	200.19

## 4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.04 mL	10.21 mL	20.43 mL
5 mM	0.41 mL	2.04 mL	4.09 mL
10 mM	0.20 mL	1.02 mL	2.04 mL
50 mM	0.04 mL	0.20 mL	0.41 mL

## 5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of “Calculator”

## 6. Recommended literature which reported protocols for in vitro and in vivo study

### In vitro study

1. Chaturvedi A, Herbst L, Pusch S, Klett L, Goparaju R, Stichel D, Kaulfuss S, Panknin O, Zimmermann K, Toschi L, Neuhaus R, Haegerbarth A, Rehwinkel H, Hess-Stumpp H, Bauser M, Bochtler T, Struys EA, Sharma A, Bakkali A, Geffers R, Araujo-Cruz MM, Thol F, Gabdoulline R, Ganser A, Ho AD, von Deimling A, Rippe K, Heuser M, Krämer A. Pan-mutant-IDH1 inhibitor BAY1436032 is highly effective against human IDH1 mutant acute myeloid leukemia in vivo. *Leukemia*. 2017 Oct;31(10):2020-2028. doi: 10.1038/leu.2017.46. Epub 2017 Jan 31. PMID: 28232670; PMCID: PMC5629366.

### In vivo study

1. Chaturvedi A, Herbst L, Pusch S, Klett L, Goparaju R, Stichel D, Kaulfuss S, Panknin O, Zimmermann K, Toschi L, Neuhaus R, Haegerbarth A, Rehwinkel H, Hess-Stumpp H, Bauser M, Bochtler T, Struys EA, Sharma A, Bakkali A, Geffers R, Araujo-Cruz MM, Thol F, Gabdoulline R, Ganser A, Ho AD, von Deimling A, Rippe K, Heuser M, Krämer A. Pan-mutant-IDH1 inhibitor BAY1436032 is highly effective against human IDH1 mutant acute myeloid leukemia in vivo. *Leukemia*. 2017 Oct;31(10):2020-2028. doi: 10.1038/leu.2017.46. Epub 2017 Jan 31. PMID: 28232670; PMCID: PMC5629366.

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## 7. Bioactivity

Biological target: BAY-1436032 is an isocitrate dehydrogenase 1 (IDH1) inhibitor.

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### In vitro activity

In vitro, BAY1436032 specifically inhibited R-2HG production and colony growth, and induced myeloid differentiation of AML (acute myeloid leukemia) cells carrying IDH1R132H, IDH1R132C, IDH1R132G, IDH1R132L and IDH1R132S mutations. In addition, the compound affected DNA methylation and attenuated histone hypermethylation.

Reference: Leukemia. 2017 Oct;31(10):2020-2028. <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5629366/>

### In vivo activity

In vivo, oral administration of BAY1436032 led to leukemic blast clearance, myeloid differentiation, depletion of leukemic stem cells and prolonged survival in two independent patient-derived xenograft IDH1 mutant AML mouse models.

Reference: Leukemia. 2017 Oct;31(10):2020-2028. <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5629366/>

*Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.*