Product data sheet



| MedKoo Cat#: 111014 | | | |
|--|--|--------------------------|--|
| Name: Obacunone | | | |
| CAS: 751-03-1 | | | |
| Chemical Formula: C ₂₆ H ₃₀ O ₇ | | | |
| Exact Mass: 454.1992 | | \ \[\bar{\parallel{1}}\] | |
| Molecular Weight: 454.519 | | _ (, \ \ \ | |
| Product supplied as: | Powder | | |
| Purity (by HPLC): | ≥ 98% | | |
| Shipping conditions | Ambient temperature |] OXÁ | |
| Storage conditions: | Powder: -20°C 3 years; 4°C 2 years. |] ' ' | |
| | In solvent: -80°C 3 months; -20°C 2 weeks. | | |

1. Product description:

Obacunone is from bark of the Chinese plant Phellodendron amurense. It exhibits anti-cancer and anti-inflammatory properties. Obacunone also significantly inhibits aromatase activity in an in vitro enzyme assay with an IC50 value of $28.04~\mu M$ and is a novel activator of Nrf2.

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 | 170.0 | 374.02 |

4. Stock solution preparation table:

| Concentration / Solvent Volume / Mass | 1 mg | 5 mg | 10 mg | | | |
|---------------------------------------|---------|----------|----------|--|--|--|
| 1 mM | 2.20 mL | 11.00 mL | 22.00 mL | | | |
| 5 mM | 0.44 mL | 2.20 mL | 4.40 mL | | | |
| 10 mM | 0.22 mL | 1.10 mL | 2.20 mL | | | |
| 50 mM | 0.04 mL | 0.22 mL | 0.44 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. Kim J, Jayaprakasha GK, Patil BS. Obacunone exhibits anti-proliferative and anti-aromatase activity in vitro by inhibiting the p38 MAPK signaling pathway in MCF-7 human breast adenocarcinoma cells. Biochimie. 2014 Oct;105:36-44. doi: 10.1016/j.biochi.2014.06.002. Epub 2014 Jun 11. PMID: 24927687.

2. Vikram A, Jayaprakasha GK, Jesudhasan PR, Pillai SD, Patil BS. Obacunone represses Salmonella pathogenicity islands 1 and 2 in an envZ-dependent fashion. Appl Environ Microbiol. 2012 Oct;78(19):7012-22. doi: 10.1128/AEM.01326-12. Epub 2012 Jul 27. PMID: 22843534; PMCID: PMC3457478.

In vivo study

1. Hu H, Wang X, Huang Y, He B, Zhu J, Sun K, Deng C, Guo Y, Hao D, Jian B. Obacunone inhibits RANKL/M-CSF-mediated osteoclastogenesis by suppressing integrin- FAK-Src signaling. Cytokine. 2023 Apr;164:156134. doi: 10.1016/j.cyto.2023.156134. Epub 2023 Feb 15. PMID: 36804257.

2. He J, Zheng L, Li X, Huang F, Hu S, Chen L, Jiang M, Lin X, Jiang H, Zeng Y, Ye T, Lin D, Liu Q, Xu J, Chen K. Obacunone targets macrophage migration inhibitory factor (MIF) to impede osteoclastogenesis and alleviate ovariectomy-induced bone loss. J Adv Res. 2023 Jan 16:S2090-1232(23)00003-6. doi: 10.1016/j.jare.2023.01.003. Epub ahead of print. PMID: 36657717.

Product data sheet



7. Bioactivity

Biological target:

Obacunone, isolated from Citrus fruits, exhibits anti-tumor activity by the induction of apoptosis.

In vitro activity

MTT assays confirmed that obacunone was strongly inhibited MCF-7 cell proliferation without affecting non-malignant breast cells. Treatment with obacunone increased apoptosis by up-regulating expression of the pro-apoptotic protein Bax and down-regulating the anti-apoptotic protein Bcl2, as well as inducing G1 cell cycle arrest. In addition, obacunone significantly inhibited aromatase activity in an in vitro enzyme assay. Exposure of MCF-7 breast cancer cells to obacunone down-regulated expression of inflammatory molecules including nuclear factor-kappa B (NF-κB) and cyclooxygenase-2 (COX-2).

Reference: Biochimie. 2014 Oct;105:36-44. https://pubmed.ncbi.nlm.nih.gov/24927687/

In vivo activity

Furthermore, in vivo administration of obacunone displayed super therapeutic effects in attenuating ovariectomy-induced bone loss in mice, as indicated by decreases in serum biomarkers of bone turnover, restoring of femur fracture maximum force, and reversing of the worsened bone-related parameters in ovariectomized animals. Taken together, these findings demonstrate that obacunone has pharmacological activities to suppress osteoclast differentiation through modulating the Integrin-FAK-Src pathway, and suggest that obacunone is a therapeutic candidate for the treatment and prevention of bone diseases such as osteoporosis.

Reference: Cytokine. 2023 Apr;164:156134. https://pubmed.ncbi.nlm.nih.gov/36804257/

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.