# Product data sheet

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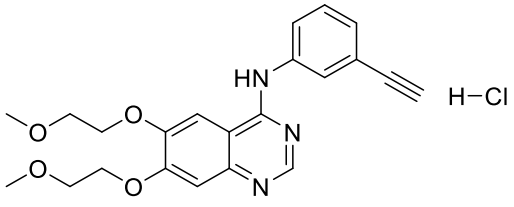
|---|---|
| MedKoo Cat#: 100300<br>Name: Erlotinib hydrochloride<br>CAS#: 183319-69-9 (HCl)<br>Chemical Formula: $C_{22}H_{24}ClN_3O_4$<br>Molecular Weight: 429.9 |  |
| Product supplied as: | Powder |
| Purity (by HPLC): | ≥ 98% |
| Shipping conditions | Ambient temperature |
| Storage conditions: | Powder: -20°C 3 years; 4°C 2 years. |
| | In solvent: -80°C 3 months; -20°C 2 weeks. |

**1. Product description:**

Erlotinib hydrochloride is the hydrochloride salt of a quinazoline derivative with antineoplastic properties. Competing with adenosine triphosphate, erlotinib reversibly binds to the intracellular catalytic domain of epidermal growth factor receptor (EGFR) tyrosine kinase, thereby reversibly inhibiting EGFR phosphorylation and blocking the signal transduction events and tumorigenic effects associated with EGFR activation.

**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 | 6.2 | 14.42 |

**4. Stock solution preparation table:**

| Concentration / Solvent Volume / Mass | 1 mg | 5 mg | 10 mg |
|---|---|---|---|
| 1 mM | 2.33 mL | 11.63 mL | 23.26 mL |
| 5 mM | 0.47 mL | 2.33 mL | 4.65 mL |
| 10 mM | 0.23 mL | 1.16 mL | 2.33 mL |
| 50 mM | 0.05 mL | 0.23 mL | 0.47 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. Marchetti S, de Vries NA, Buckle T, Bolijn MJ, van Eijndhoven MA, Beijnen JH, Mazzanti R, van Tellingen O, Schellens JH. Effect of the ATP-binding cassette drug transporters ABCB1, ABCG2, and ABCC2 on erlotinib hydrochloride (Tarceva) disposition in in vitro and in vivo pharmacokinetic studies employing Bcrp1-/-/Mdr1a/1b-/- (triple-knockout) and wild-type mice. Mol Cancer Ther. 2008 Aug;7(8):2280-7. doi: 10.1158/1535-7163.MCT-07-2250. PMID: 18723475.

2. Moyer JD, Barbacci EG, Iwata KK, Arnold L, Boman B, Cunningham A, DiOrio C, Doty J, Morin MJ, Moyer MP, Neveu M, Pollack VA, Pustilnik LR, Reynolds MM, Sloan D, Theleman A, Miller P. Induction of apoptosis and cell cycle arrest by CP-358,774, an inhibitor of epidermal growth factor receptor tyrosine kinase. Cancer Res. 1997 Nov 1;57(21):4838-48. PMID: 9354447.

In vivo study

1. Marchetti S, de Vries NA, Buckle T, Bolijn MJ, van Eijndhoven MA, Beijnen JH, Mazzanti R, van Tellingen O, Schellens JH. Effect of the ATP-binding cassette drug transporters ABCB1, ABCG2, and ABCC2 on erlotinib hydrochloride (Tarceva) disposition in in vitro and in vivo pharmacokinetic studies employing Bcrp1-/-/Mdr1a/1b-/- (triple-knockout) and wild-type mice. Mol Cancer Ther. 2008 Aug;7(8):2280-7. doi: 10.1158/1535-7163.MCT-07-2250. PMID: 18723475.

**7. Bioactivity**

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Biological target:

Erlotinib HCl (OSI-744, CP358774, NSC 718781) is an EGFR inhibitor with IC50 of 2 nM in cell-free assays, >1000-fold more sensitive for EGFR than human c-Src or v-Abl.

In vitro activity

The first indication of affinity of erlotinib for P-gp and BCRP was obtained in in vitro studies employing cells overexpressing BCRP and P-gp. A small but statistically significant difference in IC50 was found between BCRP/Bcrp1- or P-gp-overexpressing and WT cell lines, which is apparently in contrast with the high rates of transport of erlotinib observed in Transwell experiments in Bcrp1- or P-gp-overexpressing cells. A visual inspection of the plates obtained in the colony-forming assays reveals a significant difference in growth characteristics of the colonies between cell lines and at applied different concentrations of the drug. At the same erlotinib concentration, the colonies were bigger in size in the MDR1- and BCRP-expressing cells compared with WT cells, and in the same cell line, colonies were smaller (but still composed of at least 50 cells) at higher erlotinib concentrations. Therefore, the difference in the IC50 value only may not be fully representative for the effect of MDR1 or BCRP overexpression on the cytotoxicity of erlotinib.

Reference: Mol Cancer Ther. 2008 Aug;7(8):2280-7. http://mct.aacrjournals.org/cgi/pmidlookup?view=long&pmid=18723475

In vivo activity

To quantitate the effect of the absence of P-gp and Bcrp1 on the in vivo pharmacokinetics of erlotinib hydrochloride, the pharmacokinetics after p.o. and i.p. administration of the drug in WT and in Bcrp1/Mdr1a/b−/− mice was investigated. Results obtained after oral administration revealed that there is a statistically significantly increased AUC of erlotinib in triple-knockout compared with WT-mice ($P = 0.01$). In addition, the bioavailability of oral erlotinib was significantly increased in Bcrp1/Mdr1a/b−/− mice, considering also the small and nonsignificant difference in the systemic clearance of erlotinib found between Bcrp1/Mdr1a/b−/− and WT mice. Therefore, effective inhibition of P-gp/BCRP in patients may significantly increase the systemic exposure to erlotinib, assuming that these results obtained in mice are representative for the clinical situation.

Reference: Mol Cancer Ther. 2008 Aug;7(8):2280-7. http://mct.aacrjournals.org/cgi/pmidlookup?view=long&pmid=18723475