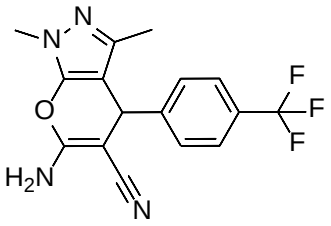
# Product data sheet

| | |
|---|---|
| MedKoo Cat#: 406646<br>Name: BQU57<br>CAS#: 1637739-82-2<br>Chemical Formula: $C_{16}H_{13}F_3N_4O$<br>Exact Mass: 334.1042<br>Molecular Weight: 334.30 |  |
| 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:**

BQU57 is a GTPase Ral inhibitor. The Ras-like GTPases RalA and RalB are important drivers of tumour growth and metastasis. Chemicals that block Ral function would be valuable as research tools and for cancer therapeutics. The binding of the RBC8 derivative BQU57 to RalB was confirmed by isothermal titration calorimetry, surface plasmon resonance and (1)H-(15)N transverse relaxation-optimized spectroscopy (TROSY) NMR spectroscopy. RBC8 and BQU57 show selectivity for Ral relative to the GTPases Ras and RhoA and inhibit tumour xenograft growth to a similar extent to the depletion of Ral using RNA interference. The utility of structure-based discovery for the development of therapeutics for Ral-dependent cancers.

**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 |
|---|---|---|
| DMF | 30.0 | 89.74 |
| DMSO | 65.33 | 195.42 |
| DMSO:PBS (pH 7.2) (1:2) | 0.33 | 0.99 |
| Ethanol | 12.50 | 37.39 |

**4. Stock solution preparation table:**

| **Concentration / Solvent Volume / Mass** | **1 mg** | **5 mg** | **10 mg** |
|---|---|---|---|
| 1 mM | 2.99 mL | 14.96 mL | 29.91 mL |
| 5 mM | 0.60 mL | 2.99 mL | 5.98 mL |
| 10 mM | 0.30 mL | 1.50 mL | 2.99 mL |
| 50 mM | 0.06 mL | 0.30 mL | 0.60 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. Thies KA, Cole MW, Schafer RE, Spehar JM, Richardson DS, Steck SA, Das M, Lian AW, Ray A, Shakya R, Knoblaugh SE, Timmers CD, Ostrowski MC, Chakravarti A, Sizemore GM, Sizemore ST. The small G-protein RalA promotes progression and metastasis of triple-negative breast cancer. Breast Cancer Res. 2021 Jun 12;23(1):65. doi: 10.1186/s13058-021-01438-3. PMID: 34118960; PMCID: PMC8196523.

In vivo study

1. Thies KA, Cole MW, Schafer RE, Spehar JM, Richardson DS, Steck SA, Das M, Lian AW, Ray A, Shakya R, Knoblaugh SE, Timmers CD, Ostrowski MC, Chakravarti A, Sizemore GM, Sizemore ST. The small G-protein RalA promotes progression and metastasis of triple-negative breast cancer. Breast Cancer Res. 2021 Jun 12;23(1):65. doi: 10.1186/s13058-021-01438-3. PMID: 34118960; PMCID: PMC8196523.

# Product data sheet

**7. Bioactivity**

Biological target: BQU57 is a GTPase Ral inhibitor with IC50s of 2.0 μM in H2122 and 1.3 μM in H358.

In vitro activity

Whether BQU57 could improve efficacy of a standard chemotherapeutic agent used to treat TNBC (triple negative breast cancer) was evaluated. MDA-MB-231 cells were treated with 100μM of BQU57 and a range of paclitaxel up to 1000nM. BQU57 had a significant additive effect with submaximal concentrations of paclitaxel (Fig. 6g).

Reference: Breast Cancer Res. 2021 Jun 12;23(1):65. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC8196523/

In vivo activity

The efficacy of BQU57 was tested in vivo by treatment of mice bearing palpable MDA-MB-231 tumors. BQU57 significantly hindered both primary tumor growth (Fig. 6d) and spontaneous lung metastasis as defined by the percent area of lung occupied by metastatic lesions (Fig. 6e). BQU57 was also tested in mice bearing patient-derived xenografts (PDX) derived from a TNBC lung metastasis. Again BQU57 significantly reduced tumor growth (Fig. 6f).

Reference: Breast Cancer Res. 2021 Jun 12;23(1):65. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC8196523/