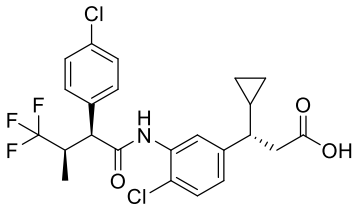
Product data sheet

MedKoo Cat#: 584817 Name: Runcaciguat CAS#: 1402936-61-1 Chemical Formula: $C_{23}H_{22}Cl_2F_3NO_3$ Exact Mass: 487.0929 Molecular Weight: 488.33	
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:

Runcaciguat, also known as BAY 1101042, is a novel, potent, and orally active sGC activator. Runcaciguat activated the sGC reporter cell line with an EC50 value of 11.2 ± 1.0 nM. Pretreatment of the sGC reporter cell line with 30 μM ODQ for 3 h resulted in an increased potency of runcaciguat (EC50 of 2.1 ± 0.07 nM), and treatment of the reporter cells with runcaciguat in combination with the NO donor S-nitroso-N-acetylpenicillamine (SNAP) (10 and 100 nM) showed additive effects. Treatment with runcaciguat resulted in maximal luminescence signals in the range of 50–60% in comparison to the sGC activator cinaciguat. Given the broad impact of oxidative stress in cardiovascular and cardiorenal diseases, runcaciguat might become a new treatment modality for a broad variety of diseases in these indication space but also beyond.

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		

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.05 mL	10.24 mL	20.48 mL
5 mM	0.41 mL	2.05 mL	4.10 mL
10 mM	0.20 mL	1.02 mL	2.05 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

Hahn MG, Lampe T, El Sheikh S, Griebenow N, Woltering E, Schlemmer KH, Dietz L, Gerisch M, Wunder F, Becker-Pelster EM, Mondritzki T, Tinel H, Knorr A, Kern A, Lang D, Hueser J, Schomber T, Benardeau A, Eitner F, Truebel H, Mittendorf J, Kumar V, van den Akker F, Schaefer M, Geiss V, Sandner P, Stasch JP. Discovery of the Soluble Guanylate Cyclase Activator Runcaciguat (BAY 1101042). J Med Chem. 2021 May 13;64(9):5323-5344. doi: 10.1021/acs.jmedchem.0c02154. Epub 2021 Apr 19. PMID: 33872507.

In vivo study

TBD

7. Bioactivity

Biological target:

A novel, potent, and orally active sGC activator.

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In vitro activity

The investigation of the structure-activity relationship allowed to improve potency and multiple solubility, permeability, metabolism, and drug-drug interactions parameters. This program resulted in the discovery of the oral sGC activator runcaciguat (compound 45, BAY 1101042). Runcaciguat is currently investigated in clinical phase 2 studies for the treatment of patients with chronic kidney disease and nonproliferative diabetic retinopathy.

Reference: Hahn MG, Lampe T, El Sheikh S, Griebenow N, Woltering E, Schlemmer KH, Dietz L, Gerisch M, Wunder F, Becker-Pelster EM, Mondritzki T, Tinel H, Knorr A, Kern A, Lang D, Hueser J, Schomber T, Benardeau A, Eitner F, Truebel H, Mittendorf J, Kumar V, van den Akker F, Schaefer M, Geiss V, Sandner P, Stasch JP. Discovery of the Soluble Guanylate Cyclase Activator Runcaciguat (BAY 1101042). J Med Chem. 2021 May 13;64(9):5323-5344. doi: 10.1021/acs.jmedchem.0c02154. Epub 2021 Apr 19. PMID: 33872507.

In vivo activity

TBD