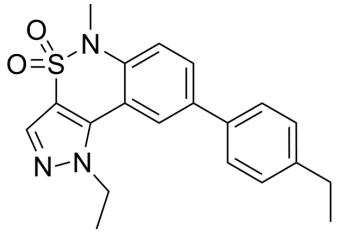
FAK inhibitor 5

Cat. No.:	HY-18928
CAS No.:	1426683-30-8
Molecular Formula:	$C_{20}H_{21}N_3O_2S$
Molecular Weight:	367.46
Target:	FAK
Pathway:	Protein Tyrosine Kinase/RTK
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	FAK inhibitor 5 (compound 2) is a novel allosteric FAK inhibitor, with IC_{50} values in the low micromolar range[1].
IC_{50} & Target	1.6 μM (pre-incubation 5 min ATP 0.5 μM), 1.3 μM (pre-incubation 60 min ATP 0.5 μM), 3.0 μM (pre-incubation 5 min ATP 1000 μM), 1.0 μM (pre-incubation 60 min ATP 1000 μM).
In Vitro	The binding interactions between FAK inhibitor 5 (compound 2) in the FAK allosteric site is mostly hydrophobic in nature. Exposure of the allosteric pocket by the dramatic movement of Ile547 is accompanied by an equally significant movement of Arg550 in toward the allosteric binding site, where it packs along the tricyclic core of compounds 2. Notably, the terminal ethylphenyl group of compounds 2 occupies the DFG-in pocket, thereby dislodging Phe565 and enabling the structural rearrangement of the activation loop and observed occlusion of the FAK active site[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Applied Materials Today. 27, June 2022, 101465.

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REFERENCES

[1]. Iwatani M, et al. Discovery and characterization of novel allosteric FAK inhibitors. Eur J Med Chem. 2013 Mar;61:49-60.

Caution: Product has not been fully validated for medical applications. For research use only.

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