# Keap1-Nrf2-IN-13

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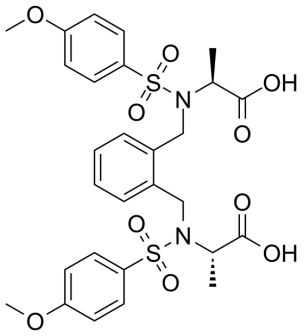
| **Cat. No.:** | HY-150579 |
| **CAS No.:** | 2456294-92-9 |
| **Molecular Formula:** | $C_{28}H_{32}N_2O_{10}S_2$ |
| **Molecular Weight:** | 620.69 |
| **Target:** | Keap1-Nrf2 |
| **Pathway:** | NF-κB |
| **Storage:** | Please store the product under the recommended conditions in the Certificate of Analysis. |



## BIOLOGICAL ACTIVITY

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| **Description** | Keap1-Nrf2-IN-13 is a Keap1-Nrf2 protein–protein interaction (PPI) inhibitor with an $IC_{50}$ value of 0.15 μM. Keap1-Nrf2-IN-13 has strong binding affinities to the Keap1 protein by forming hydrogen bond with the key polar residues (Asn414, Arg415, Arg483, Gln530). Keap1-Nrf2-IN-13 can be used in the research of oxidative stress-related and inflammatory diseases, including pulmonary fibrosis, chronic obstructive pulmonary disorder (COPD) and cancers[1]. |
| **$IC_{50}$ & Target** | IC50: 0.15 μM (Keap1-Nrf2 PPI)[1] |
| **In Vitro** | Keap1-Nrf2-IN-13 (compound 21a, 0.5-50 μM) has inhibitory effect against Keap1-Nrf2 protein–protein interaction (PPI) with an $IC_{50}$ value of 0.15 μM (fluorescence polarization (FP) assay)[1].<br>Keap1-Nrf2-IN-13 (0.1 mM, 90 min) has metabolic stability in the presence of human liver microsomes[1].<br>Keap1-Nrf2-IN-13 forms hydrogen bond interactions with the key polar residues (Asn414, Arg415, Arg483, Gln530), resulting in strong binding affinities to the Keap1 protein (docking assay)[1].<br>MCE has not independently confirmed the accuracy of these methods. They are for reference only. |

## REFERENCES

[1]. [1] Dhulfiqar Ali Abed, et al. Discovery of disubstituted xylylene derivatives as small molecule direct inhibitors of Keap1-Nrf2 protein-protein interaction. Bioorg Med Chem. 2020 Mar 15;28(6):115343.



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