



## Product Information

### Integrin inhibitor, Carotegrast, Purity $\geq 98\%$

**Cat. No.:** X24-08-YM314

**Size:** 1 mg; 5 mg; 10 mg; 50 mg

**CAS Number:** 401904-75-4

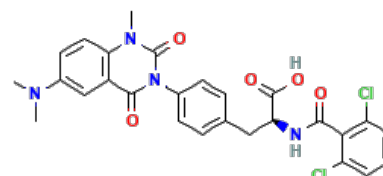
**Compound CID:** 10120218

**Synonym:** 401904-75-4;

(2S

)-2-[(2,6-Dichlorobenzoyl)amino]-3-[4-[6-(dimethylamino)-1-methyl-2,4-dioxoquinazolin

-3-yl]phenyl]propanoic acid



**This product is for research use only and is not intended for diagnostic use.**

#### Product Information

|                          |                                                                                                                                                                                                  |
|--------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Description</b>       | Carotegrast is an effective cytoskeleton inhibitor, that has the ability to prevent the pathway of cytoskeletal signaling by inhibiting integrin.                                                |
| <b>Molecular Weight</b>  | 555.41                                                                                                                                                                                           |
| <b>Molecular Formula</b> | C <sub>27</sub> H <sub>24</sub> Cl <sub>2</sub> N <sub>4</sub> O <sub>5</sub>                                                                                                                    |
| <b>IUPAC Name</b>        | (2S<br>)-2-[(2,6-Dichlorobenzoyl)amino]-3-[4-[6-(dimethylamino)-1-methyl-2,4-dioxoquinazolin-3-yl]phenyl]propanoic acid                                                                          |
| <b>InChI</b>             | InChI=1S/C27H24Cl2N4O5/c1-31(2)17-11-12-22-18(14-17)25(35)33(27(38)32(22)3)16-9-7-15(8-10-16)13-21(26(36)37)30-24(34)23-19(28)5-4-6-20(23)29/h4-12,14,21H,13H2,1-3H3,(H,30,34)(H,36,37)/t21-m/s1 |
| <b>InChI Key</b>         | QJZRFPJCWMNVAV-HHHXNRCGSA-N                                                                                                                                                                      |
| <b>Canonical SMILES</b>  | CC1=CC=C(C=C1)C(=O)N(CCCN)C(C2=NC3=C(C=CC(=C3)Cl)C(=O)N2CC4=CC=CC=C4)C(C)C                                                                                                                       |
| <b>Isomeric SMILES</b>   | CC1=CC=C(C=C1)C(=O)N(CCCN)[C@@H](C2=NC3=C(C=CC(=C3)Cl)C(=O)N2CC4=CC=CC=C4)C(C)C                                                                                                                  |
| <b>Form</b>              | Lyophilized powder                                                                                                                                                                               |
| <b>Purity</b>            | $\geq 98\%$                                                                                                                                                                                      |
| <b>Titer</b>             | Free from inappropriate visible particulates, foreign matter, discoloration, or other defects                                                                                                    |
| <b>Stability</b>         | In its lyophilized form, the chemical remains stable for 36 months.                                                                                                                              |
| <b>Quality Level</b>     | Research grade                                                                                                                                                                                   |



---

**Applications**

Carotegrast is a cytoskeletal signaling inhibitor that can be studied extensively for its potential therapeutic applications in the treatment of inflammatory and autoimmune diseases by blocking integrin  $\alpha 4 \beta 1$ -mediated immune cell adhesion and migration.

---

**Storage**

Store at -20°C, and keep desiccated.

---