

Product Data Sheet

Product Name: AB-FUBINACA metabolite 2B

Cat. No.: GC40863

Chemical Properties

Cas. No. 2460433-24-1

Chemical Name 4-amino-3-(1-(4-fluorobenzyl)-1H-indazole-3-carboxamido)-2-methyl-4-oxobutanoic acid

SMILES O=C(NC(C(N)=O)C(C)C(O)=O)C1=NN(CC2=CC=C(F)C=C2)C3=C1C=CC=C3

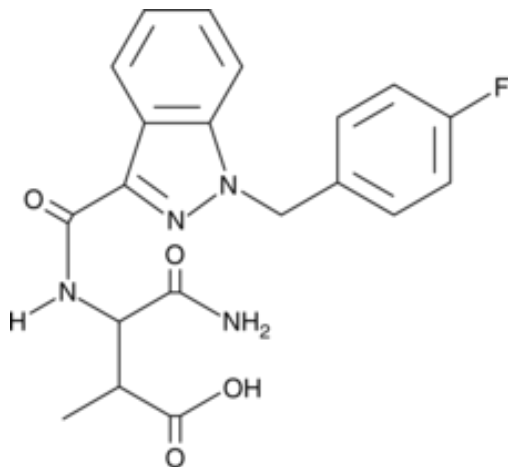
Formula C₂₀H₁₉FN₄O₄ M.Wt 398.4

Solubility DMF: 20 mg/ml, DMF:PBS(pH 7.2) (1:1): 0.5 mg/ml, DMSO: 10 mg/ml Storage Store at -20°C

General tips For obtaining a higher solubility, please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution: ship with blue ice. All other available size: ship with RT, or blue ice upon request.

Structure



Background

AB-FUBINACA is an indazole-based synthetic cannabinoid (CB) that shows high affinity for the CB1 receptor ($K_i = 0.9$ nM). [1] [2] AB-FUBINACA metabolite 2B is an expected carboxy metabolite of AB-FUBINACA, based on the major metabolites produced from similar synthetic CBs in humans. [3] [4] AB-FUBINACA metabolite 2B is a single diastereomer, but its relative stereochemistry is unknown.

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

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The other diastereomer, AB-FUBINACA metabolite 2A, is sold as . The physiological and toxicological properties of this compound are not known. This product is intended for forensic and research applications.

Reference:

- [1]. Uchiyama, N., Matsuda, S., Wakana, D., et al. New cannabimimetic indazole derivatives, N-(1-amino-3-methyl-1-oxobutan-2-yl)-1-pentyl-1H-indazole-3-carboxamide (AB-PINACA) and N-(1-amino-3-methyl-1-oxobutan-2-yl)-1-(4-fluorobenzyl)-1H-indazole-3-carboxamide (AB-FUBINACA) identified as designer drugs in illegal products. *Forensic Toxicol.* 31(1), 93-100 (2013).
- [2]. Buchler, I.P., Hayes, M.J., Hedge, S.G., et al. Indazole derivatives. 1-283 (2009).
- [3]. Sobolevsky, T., Prasolov, I., and Rodchenkov, G. Detection of JWH-018 metabolites in smoking mixture post-administration urine. *Forensic Sci. Int.* 200(1-3), 141-147 (2010).
- [4]. Moran, C.L., Le, V.H., Chimalakonda, K.C., et al. Quantitative measurement of JWH-018 and JWH-073 metabolites excreted in human urine. *Anal. Chem.* 83(11), 4228-4236 (2011).

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