

Short Communication for the Analysis of 4F-MDMB-BINACA

Date: May 2020

Synonyms: 4F-MDMB-BUTINACA

Methyl 2-[[1-(4-fluorobutyl)indazole-3-carbonyl]amino]-3,3dimethyl-butanoate

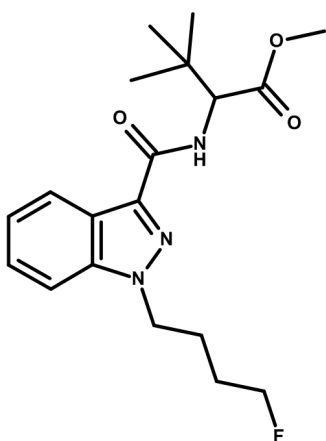
Methyl (S)-2-(1-(4-fluorobutyl)-1H-indazole-3-carboxamido)-3,3dimethylbutanoate

Methyl (2S)-2-{{1-(4-fluorobutyl)-1H-indazole-3-carbonyl}amino}-

3,3dimethylbutanoate

N-[[1-(4-Fluorobutyl)-1H-indazole-3-yl]carbonyl]-3-methyl-L-valine, methyl ester

Structure:



Formula: C₁₉H₂₆FN₃O₃

Molecular Weight (nominal mass): 363.43

Theoretical M+H accurate mass: 364.2031

Pharmacological Drug Class: Synthetic cannabinoid

Suggested LOD: 0.1 ng/mL

Suggested LOQ: 0.1 ng/mL

4F-MDMB-BINACA is a synthetic cannabinoid with an indazole core and fluorinated butyl chain as opposed to the fluorinated pentyl chain of 5F-MDMB-PINACA (5F-ADB). 4F-MDMB-BINACA was first identified in seized material and biological fluid since November 2018 in Europe and the USA with increasing detections throughout 2019 and into 2020. It is encountered similar to other synthetic cannabinoids.

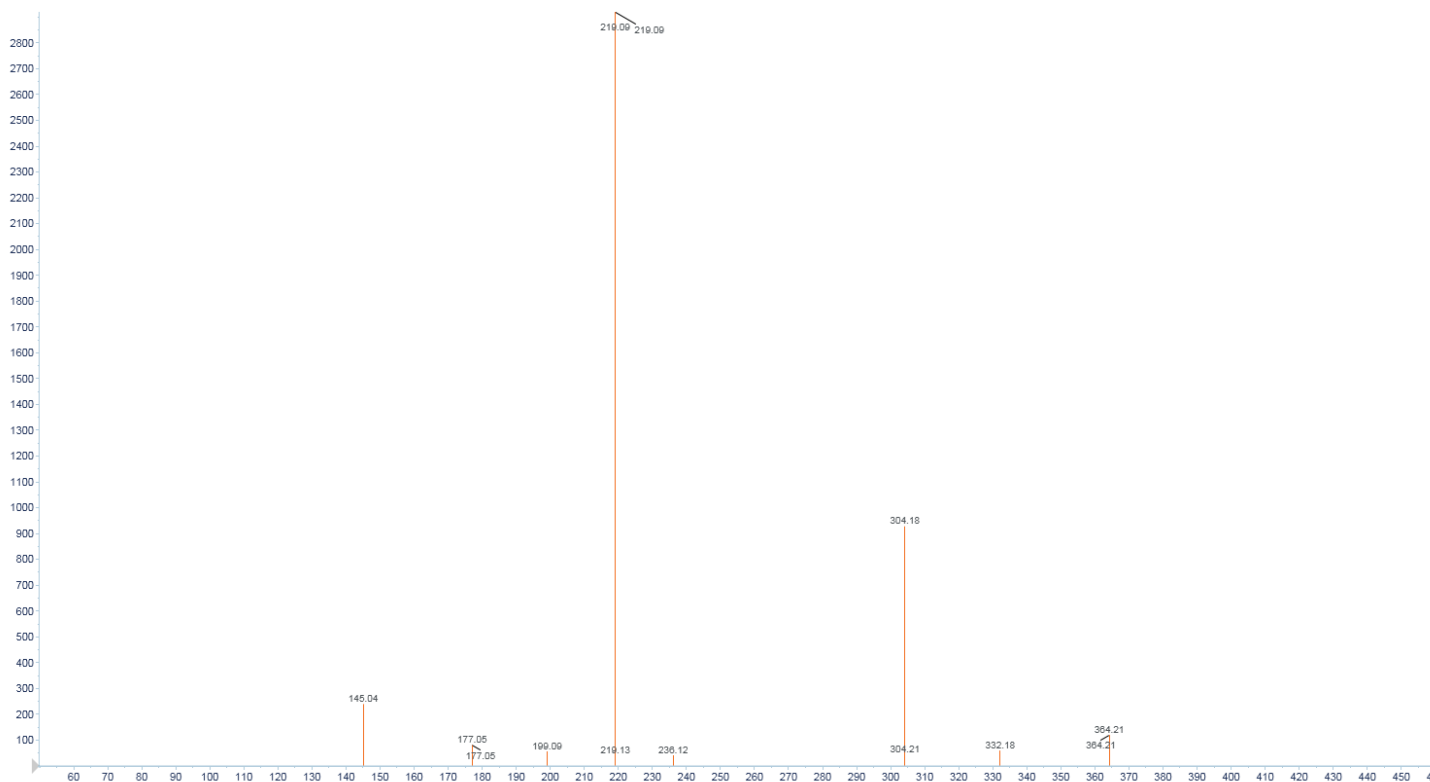
In 2019, the 42nd meeting of the World Health Organization Expert Committee on Drug Dependence critically reviewed 4F-MDMB-BINACA

(https://www.who.int/medicines/access/controlled-substances/Final_4F-MDMB-BINACA.PDF?ua=1).

At its meeting in March 2020, the Commission for Narcotic Drugs voted to place 4F-MDMB-BINACA under international control as a Schedule II substance in the 1971 Convention on Psychotropic Substances.

Although detected, there are no current reports of 4F-MDMB-BINACA concentrations in biological fluid. For limit of detection and quantitation purposes, published concentrations for 5F-MDMB-PINACA detection and measurement may apply. Studies have demonstrated that the primary metabolite of 4F-MDMB-BINACA is the ester hydrolysis metabolite as for other synthetic cannabinoids with $-OCH_3$ at the head (e.g. 5F-MDMB-PINACA). The ester metabolite of 4F-MDMB-BINACA (M+H, 350.1874) and 5F-MDMB-PINACA share common fragments and may have very similar retention times, but researchers have identified a specific 4F-MDMB-BINACA ester metabolite product ion of 290.0928 (M+H) that incorporates the fluoro-butyl chain.

LC-MS Spectrum:



[source: Sciex X500R , Travis County Medical Examiner]

References:

- Haschimi B, Mogler L, Halter S, Giorgetti A, Schwarze B, Westphal F, Fischmann S, Auwärter V. Detection of the recently emerged synthetic cannabinoid 4F-MDMB-BINACA in "legal high" products and human urine specimens. *Drug Test Anal.* (2019) 11(9):1377-1386
- Krotulski AJ, Mohr ALA, Kacinko SL, Fogarty MF, Shuda SA, Diamond FX, Kinney WA, Menendez MJ, Logan BK. 4F-MDMB-BINACA: A New Synthetic Cannabinoid Widely Implicated in Forensic Casework. *J Forensic Sci.* (2019) 64(5):1451-1461