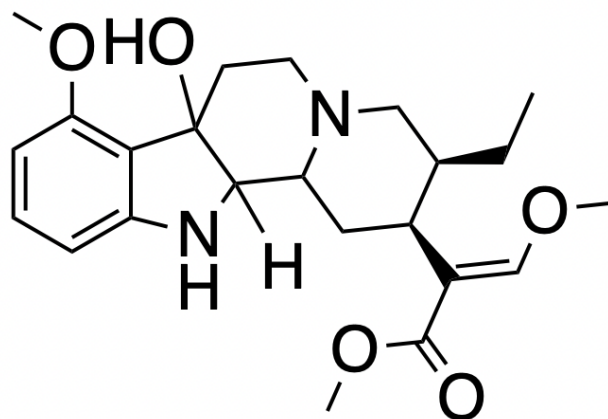


MGM-15 (C₂₃H₃₂N₂O₅)



MW: 416.51 g/ mol

CAS Registry Number

1158901-38-2

CAS Name

Indolo[2,3-*a*]quinolizine-2-acetic acid,
3-ethyl-1,2,3,4,6,7,7a,12,12a,12b-decahydro-7a-hydroxy-8-methoxy- α -(methoxymethylene)-, methyl ester, ($\alpha E, 2S, 3S, 7aS, 12aR, 12bS$)- (ACI)

Canonical SMILES

O=C(OC)C(=COC)C1CC2N(CCC3(O)C=4C(OC)=CC=CC4NC23)CC1CC

Isomeric SMILES

O[C@@]12C=3C(N[C@@]1([C@]4(N(CC2)C[C@@H](CC)[C@@H](\C(\C(OC)=O)=C/OC)C4)[H])[H])=CC=CC3OC

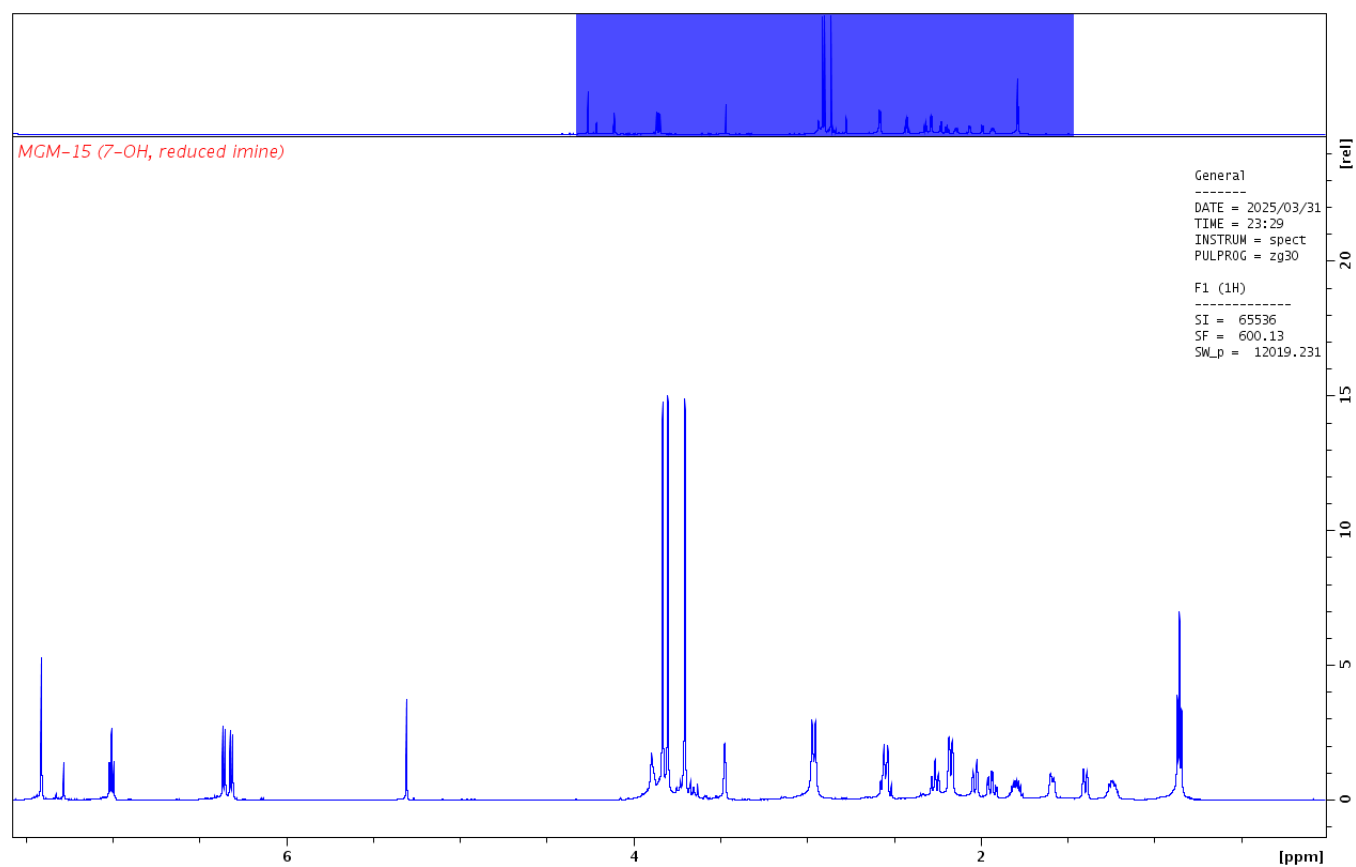
InChI

InChI=1S/C23H32N2O5/c1-5-14-12-25-10-9-23(27)20-17(7-6-8-19(20)29-3)24-21(23)18(25)11-15(14)16(13-28-2)22(26)30-4/h6-8,13-15,18,21,24,27H,5,9-12H2,1-4H3/b16-13+/t14-,15+,18+,21-,23+/m1/s1

InChI Key

QXFXDJATKPXTFF-LIMHOZK TSA-N

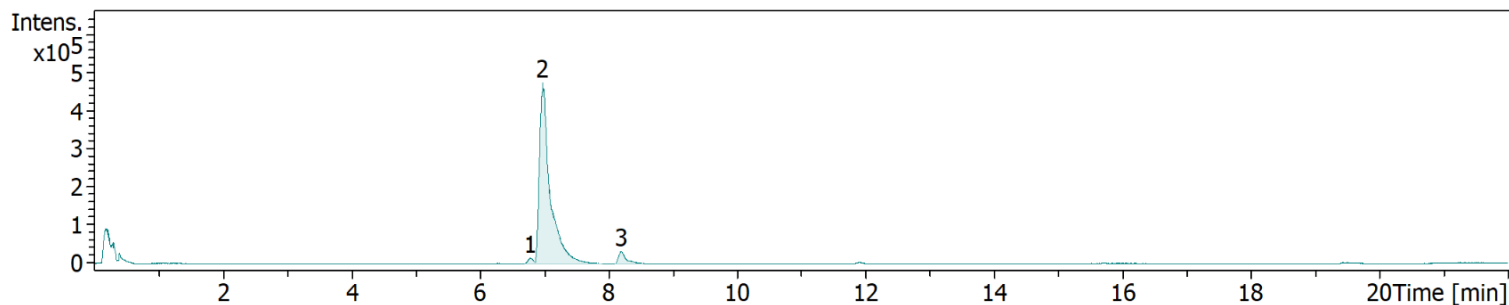
1H NMR Analysis



UPLC-MS Analysis

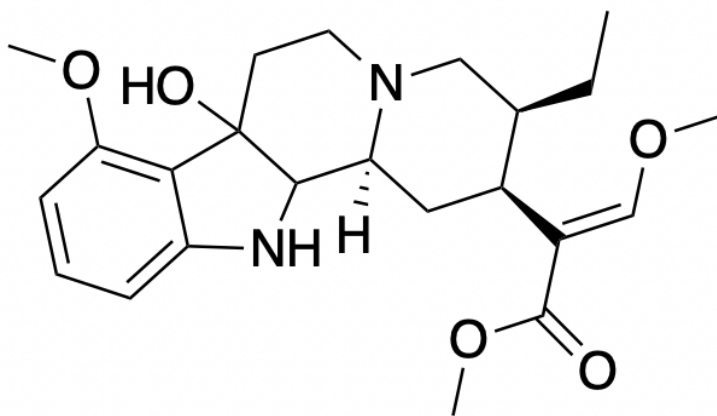
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.2 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	220 °C
Scan Begin	20 m/z	Set End Plate Offset	-500 V	Set Dry Gas	10.0 l/min
Scan End	1300 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	RT [min]	Area	Int. Type	I	S/N	Trace	Max. m/z	FWHM [min]
1	6.8	75215	Manual	14919	87.6	BPC +All MS	415.2230	0.1
2	7.0	5401821	Manual	474327	2938.1	BPC +All MS	417.2381	0.1
3	8.2	250549	Manual	31903	195.3	BPC +All MS	399.2279	0.1

MGM-15

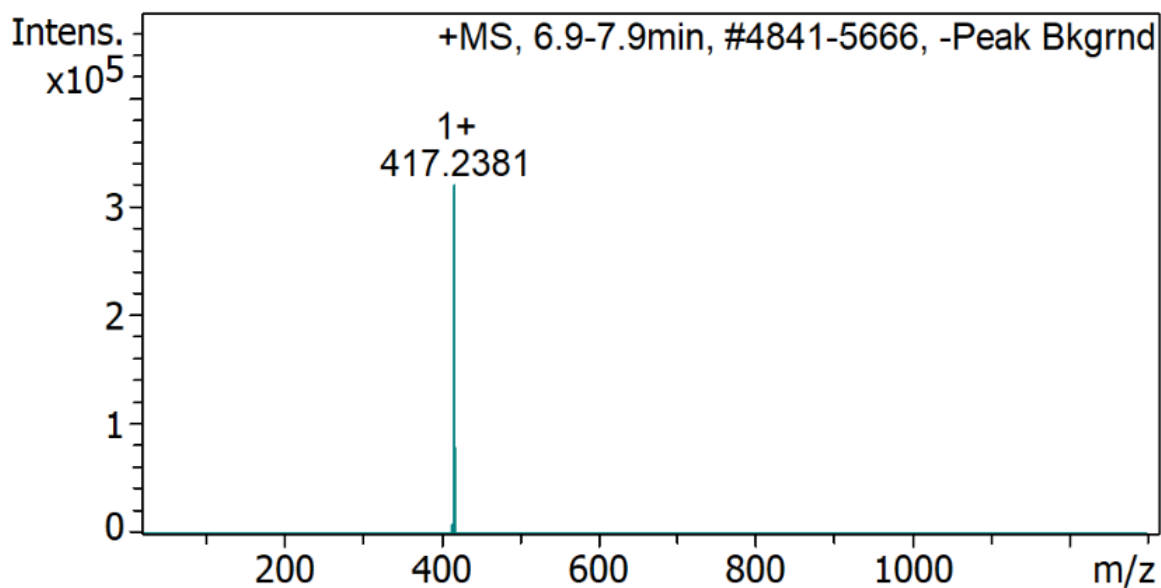


Chemical Formula: C₂₃H₃₂N₂O₅

Molecular Weight: 416.52

Expected m/z ~ 417.2

Cmpd 2, 7.0 min



#	m/z	Res.	S/N	I	I %	FWHM
1	209.1228	26450	6.3	286	0.1	0.0079
2	387.2282	31824	17.0	773	0.2	0.0122
3	415.2229	31143	181.4	8262	2.6	0.0133
4	416.2267	29910	24.6	1120	0.3	0.0139
5	417.2381	43929	7031.0	320211	100.0	0.0095
6	417.3924	34292	108.9	4957	1.5	0.0122
7	417.4936	33258	45.9	2088	0.7	0.0126
8	418.2416	40482	1735.3	79032	24.7	0.0103
9	419.2445	30744	237.9	10834	3.4	0.0136
10	420.2476	30846	10.8	493	0.2	0.0136

1. Matsumoto K, Narita M, Muramatsu N, Nakayama T, Misawa K, Kitajima M, Tashima K, Devi LA, Suzuki T, Takayama H, Horie S. Orally active opioid μ/δ dual agonist MGM-16, a derivative of the indole alkaloid mitragynine, exhibits potent antiallodynic effect on neuropathic pain in mice. J Pharmacol Exp Ther. 2014 Mar;348(3):383-92. doi: 10.1124/jpet.113.208108. Epub 2013 Dec 17. Erratum in: J Pharmacol Exp Ther. 2019 Apr;369(1):142. doi: 10.1124/jpet.112.208108err. PMID: 24345467; PMCID: PMC6067406.

HEAVY METALS	Action Level	Result
Lead (Pb)	15 ppb	Not Detected
Mercury (Hg)	2 ppb	Not Detected
Cadmium (Cd)	5 ppb	Not Detected
Arsenic (As)	10 ppb	Not Detected
Chromium (Cr)	100 ppb	Not Detected
Nickel (Ni)	100 ppb	Not Detected
Cobalt (Co)	100 ppb	Not Detected
Copper (Cu)	1300 ppb	Not Detected
Zinc (Zn)	5000 ppb	Not Detected
Iron (Fe)	300 ppb	Not Detected
Thallium (Tl)	2 ppb	Not Detected
Aluminum (Al)	200 ppb	Not Detected

* Based on South Carolina Action Limits

Residual Solvents	Action Level	Quantitative Result
Benzene	2 ppm	Not Detected
Carbon Tetrachloride	4 ppm	Not Detected
Chloroform	80 ppm	Not Detected
Methanol	3000 ppm	Not Detected
Acetonitrile	410 ppm	Not Detected
Tetrahydrofuran	720 ppm	Not Detected
N-Hexane	290 ppm	Not Detected
Ethyl Acetate	5000 ppm	Not Detected
Ethanol	5000 ppm	Not Detected
Acetone	5000 ppm	Not Detected
Isopropyl Alcohol	5000 ppm	Not Detected
Dichloromethane	600 ppm	Not Detected

Residual Solvents analysis is performed using Gas Chromatography / Mass Spectrometry. *Based on SC Action Limits.