

Famprofazone

CAS Registry No.: 22881-35-2

Formal Name: 4-isopropyl-1-methyl-5-((methyl(1-phenylpropan-2-yl)amino)methyl)-2-phenyl-1,2-dihydro-3H-pyrazol-3-one

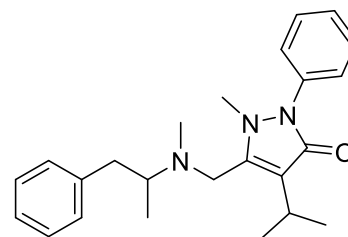
EUBOPEN ID: EUB0002359a

Molecular Formula: C₂₄H₃₁N₃O

Molecular Weight: 377.53 g/mol

Smiles: CC(C)C1=C(N(N(C1=O)C2=CC=C(C=C2)C)CN(C)C(C)CC3=CC=CC=C3

Recommended concentration: 1 μM

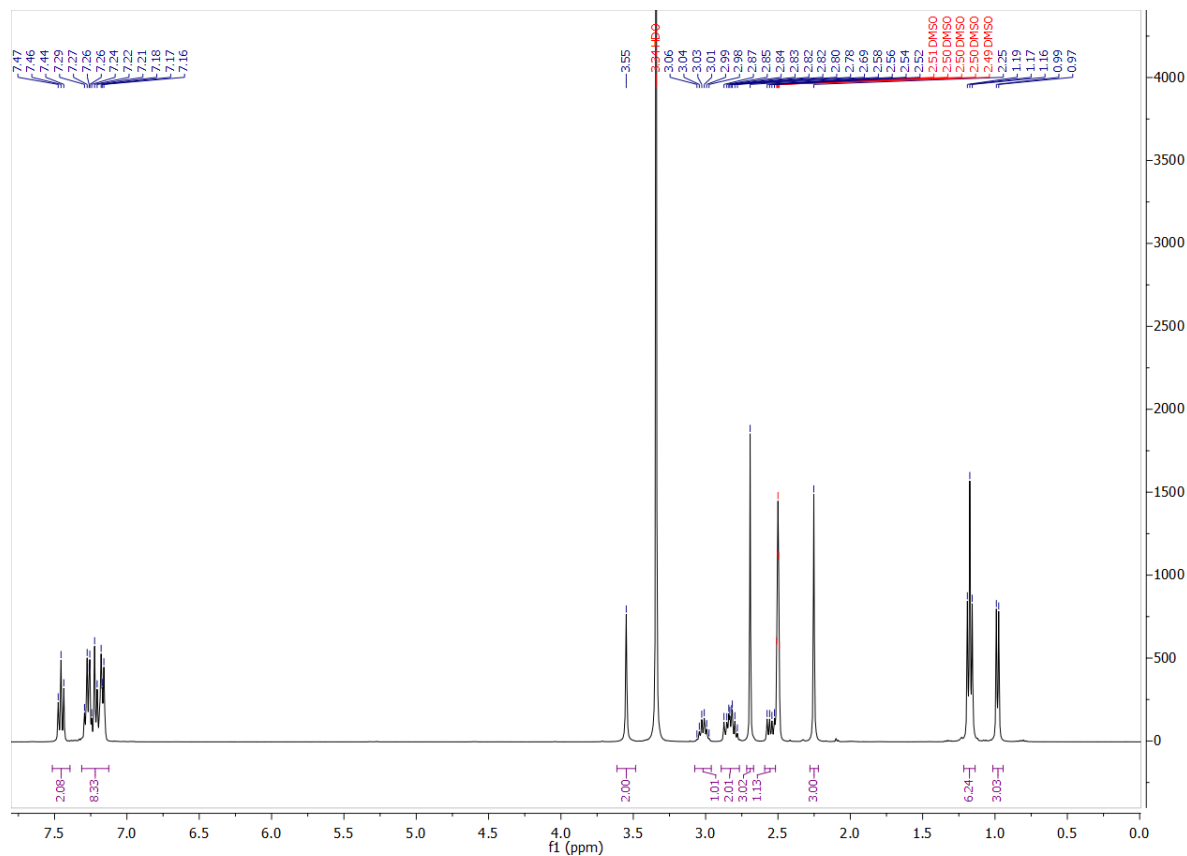


Biological activity

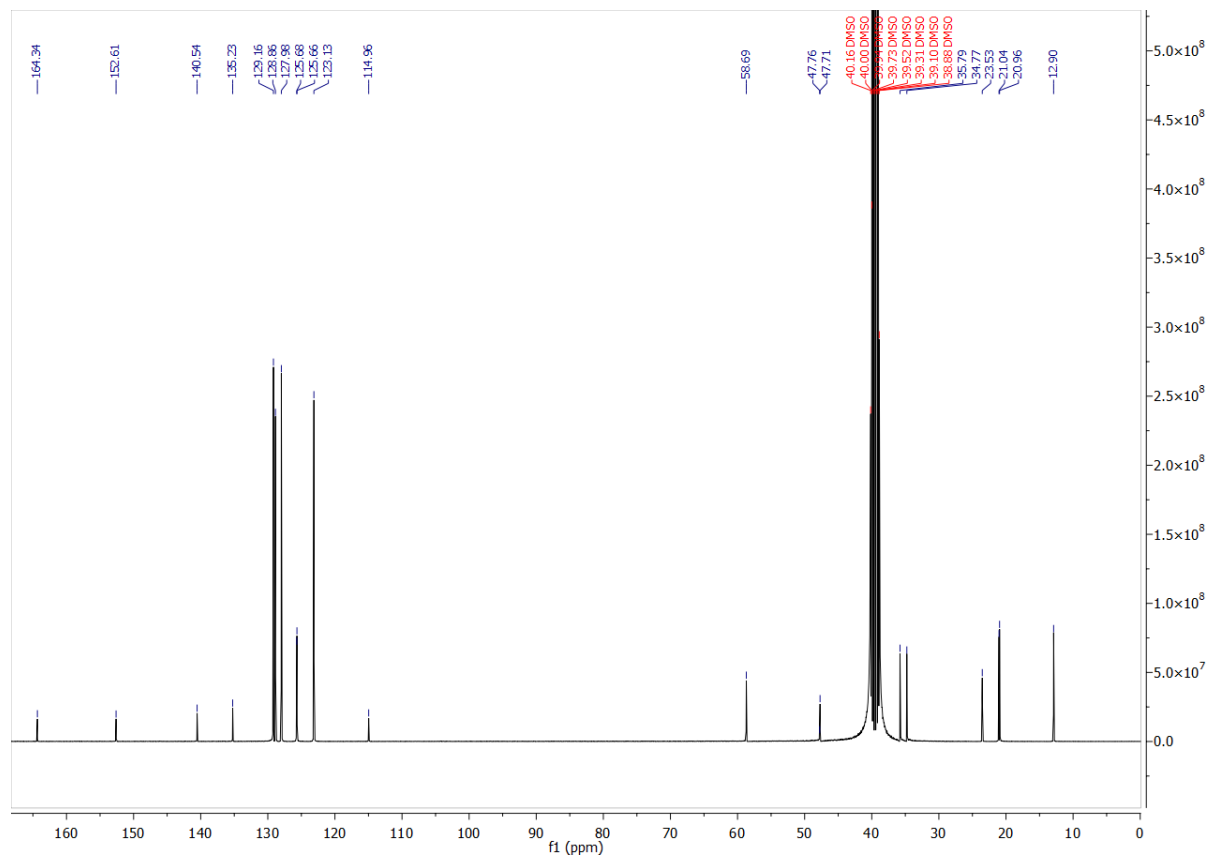
		Type	IC ₅₀ /EC ₅₀ [μM]	Reference
Main NR target:	NR112 (PXR)	Agonist	0.13	inhouse
NR off-target:				

Identity

¹H NMR



¹³C NMR



COMPOUND INFORMATION

Purity

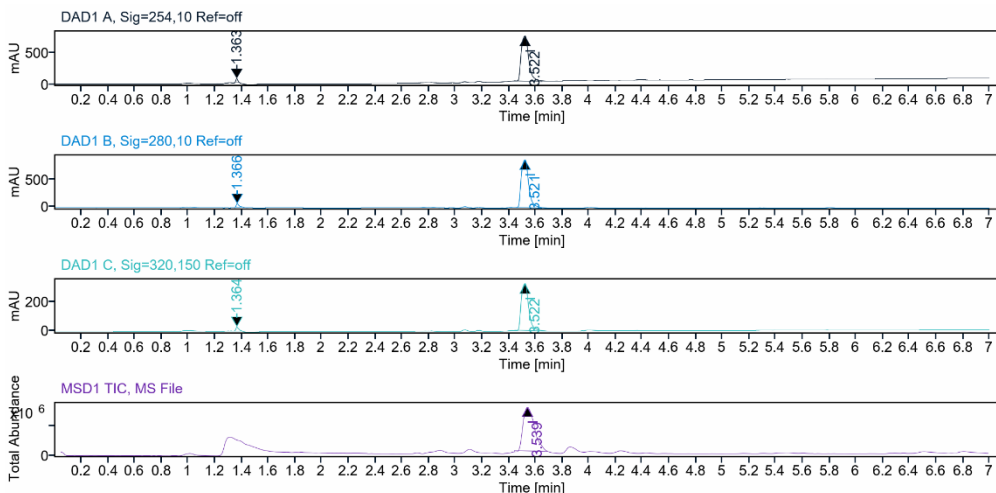
Data file: W:\analytical_LCMS_DATA\Sandra\Famprofazone (1) 2024-02-14 16-06-42.D
Sample name: Famprofazone
Description:
Sample amount: 0.000 **Sample type:** Sample
Instrument: LCMS test **Location:** D2F-D1
Injection date: 2024-02-14 16:09:22+01:00 **Injection:** 1 of 1
Injection volume: 6.000
Acq. method: FAST_Nonpolar_General_Method_MS-PosScan-100-1000.M
Analysis method: SR_03_25_RP-0,5ml_7.5µL_GRAD - 7min_284_280 nm_INJPROG_low.M

Module	Type	Part. No.	Serial No.	Firmware
Agilent G6125B MSD	Detector	G6125B	<undef>	3.02.50
Quat. Pump	Pump	G7104C	DEAGZ01778	B.07.35 [0002]
Column Comp.	Column compartment	G7116A	DEAEM06531	D.07.35 [0002]
DAD	Detector	G7117C	DEAEK07274	D.07.35 [0002]
Multisampler	Auto sampler	G7167A	DEAGY01736	D.07.38 [0003]

Results

Sample Name Famprofazone

Chromatograms



Sample Purity

Signal Description DAD1 A, Sig=254,10 Ref=off

Sample Name	Name	RT	Width	Area	Area%	Height
Famprofazone		1.363	0.016	62.6505	2.14	64.5794
Famprofazone		3.522	0.060	2868.1563	97.86	738.2081

Max Area% 97.862

UV Signal Purity>95% **Pass**

Signal Description DAD1 B, Sig=280,10 Ref=off

Sample Name	Name	RT	Width	Area	Area%	Height
Famprofazone		1.366	0.021	90.9742	2.65	63.8089
Famprofazone		3.521	0.059	3347.0217	97.35	875.5484

Max Area% 97.354

UV Signal Purity>95% **Pass**

COMPOUND INFORMATION

Signal Description DAD1 C, Sig=320,150 Ref=off

Sample Name	Name	RT	Width	Area	Area%	Height
Famprofazone		1.364	0.022	40.3872	3.12	29.0652
Famprofazone		3.522	0.060	1252.8397	96.88	329.1352

Max Area% 96.877

UV Signal Purity>95% **Pass**

UV Apex Spectra

RT:

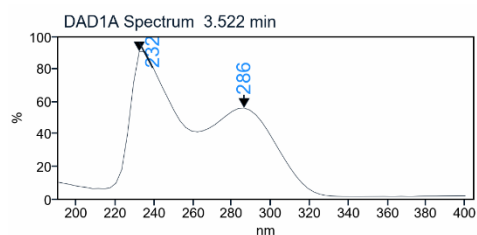
3.522

Sample Name:

Famprofazone

Signal Name:

DAD1A



MSD Apex Spectra

RT:

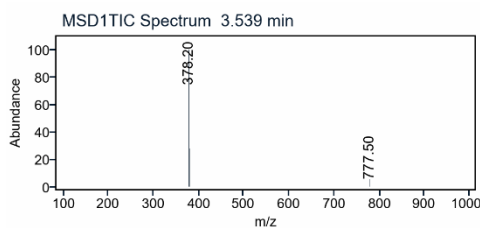
3.539

Sample Name:

Famprofazone

Signal Name:

MSD1TIC



Biological activity

Famprofazone
PXR - EC₅₀ 0.13 ± 0.4 μM
1.8 ± 0.7 fold activation

