

## Oxatomide

**CAS Registry No.:** 60607-34-3

**Formal Name:** 1-(3-(4-benzhydrylpiperazin-1-yl)propyl)-1,3-dihydro-2H-benzo[d]imidazol-2-one

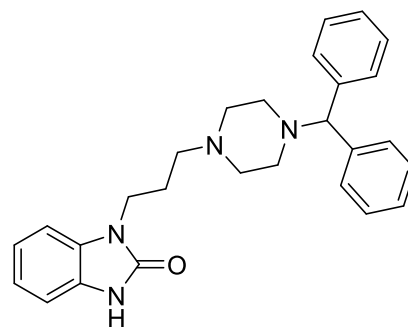
**EUBOPEN ID:** EUB0002358a

**Molecular Formula:** C<sub>27</sub>H<sub>30</sub>N<sub>4</sub>O

**Molecular Weight:** 426.56 g/mol

**Smiles:** O=c1[nH]c2ccccc2n1CCCN1CCN(C(c2ccccc2)c2ccccc2)CC1

**Recommended concentration:** 10 μM

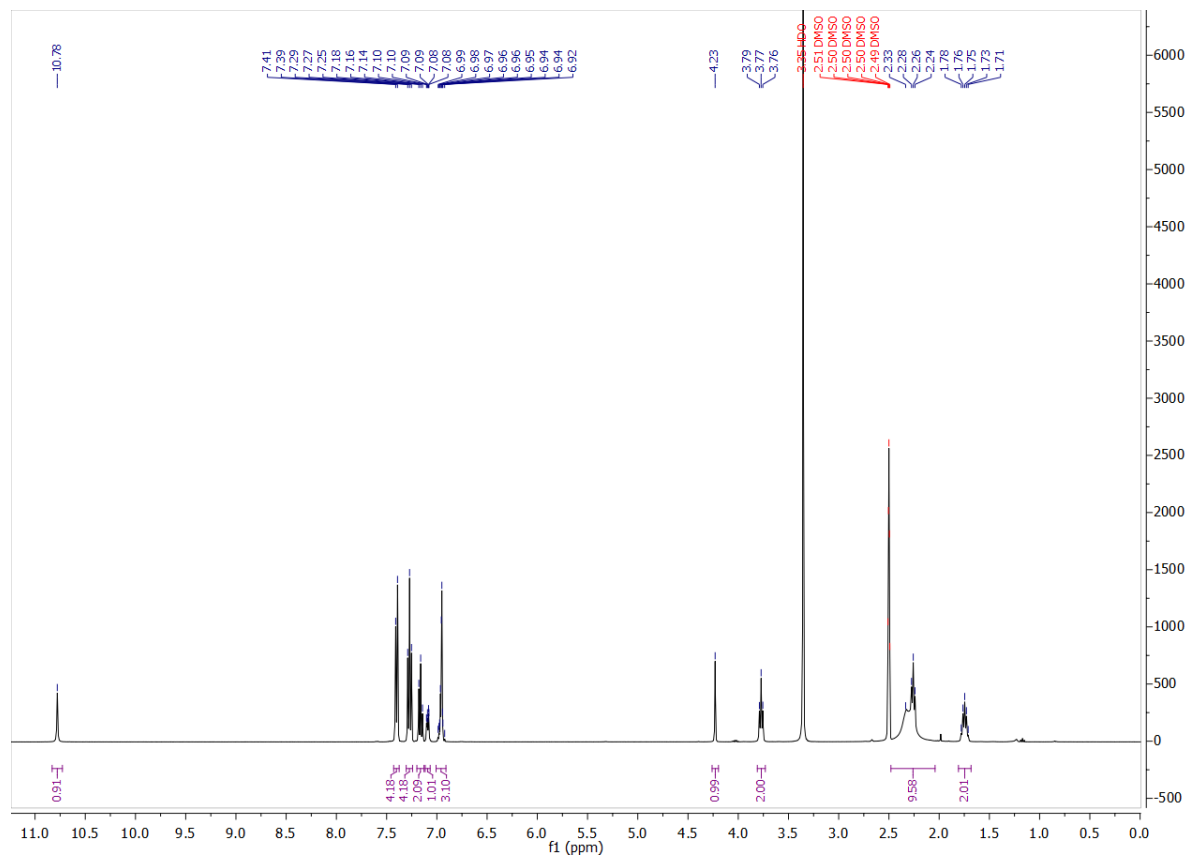


### Biological activity

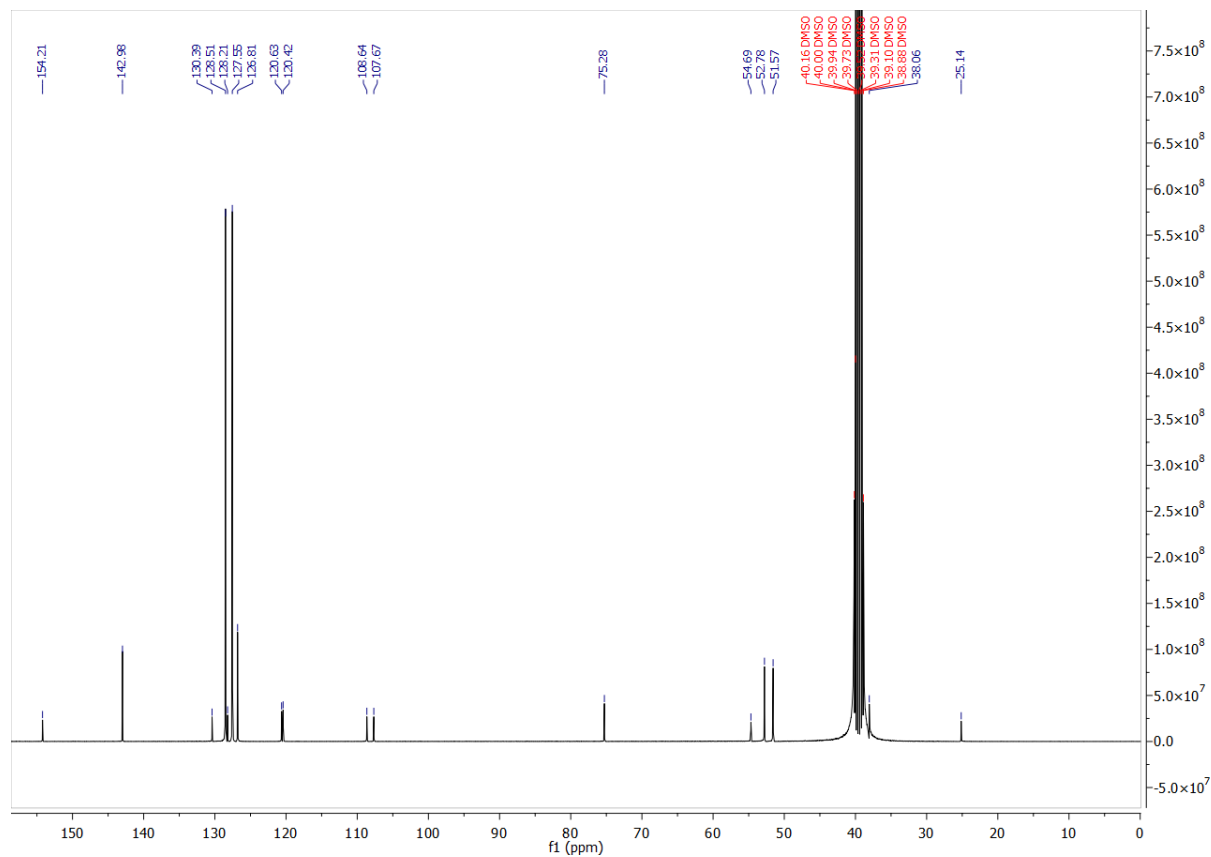
		Type	IC <sub>50</sub> /EC <sub>50</sub> [μM]	Reference
Main NR target:	NR112 (PXR)	Agonist	6	inhouse
NR off-target:				

## Identity

### <sup>1</sup>H NMR



### <sup>13</sup>C NMR



# COMPOUND INFORMATION

## Purity

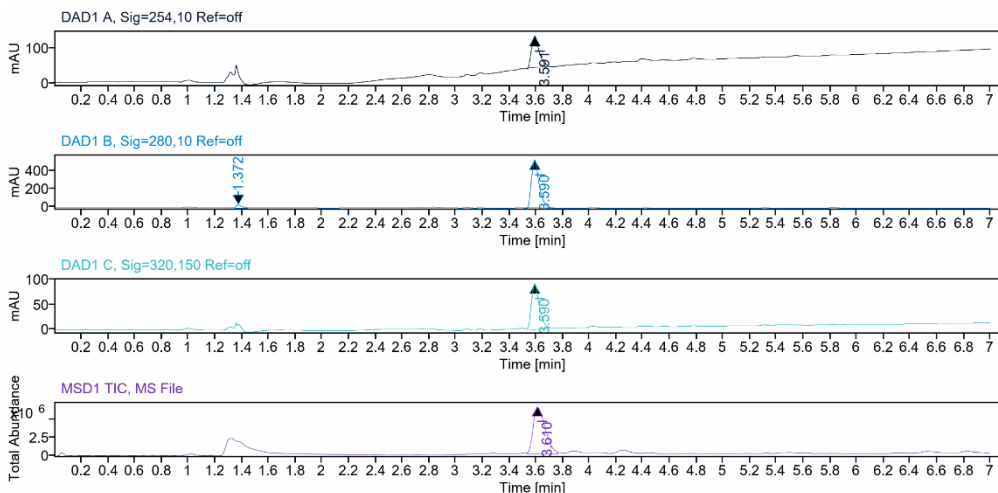
**Data file:** W:\analytical\_LCMS\_DATA\Sandra\Oxatomide (1) 2024-02-14 16-07-32.D  
**Sample name:** Oxatomide  
**Description:**  
**Sample amount:** 0.000 **Sample type:** Sample  
**Instrument:** LCMS test **Location:** D2F-D3  
**Injection date:** 2024-02-14 16:44:24+01:00 **Injection:** 1 of 1  
**Injection volume:** 8.000  
**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 Oxatomide

### Chromatograms



### Sample Purity

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

Sample Name	Name	RT	Width	Area	Area%	Height
Oxatomide		3.591	0.061	353.3834	100.00	90.8205

Max Area% 100.000

UV Signal Purity>95% **Pass**

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

Sample Name	Name	RT	Width	Area	Area%	Height
Oxatomide		1.372	0.049	112.9369	5.26	36.4522
Oxatomide		3.590	0.060	2034.6965	94.74	518.3704

Max Area% 94.741

UV Signal Purity>95% **Fail**

# COMPOUND INFORMATION

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

Sample Name	Name	RT	Width	Area	Area%	Height
Oxatomide		3.590	0.063	376.0159	100.00	92.4773

Max Area% 100.000

UV Signal Purity>95% **Pass**

## UV Apex Spectra

RT:

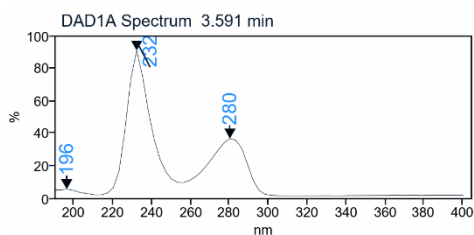
3.591

Sample Name:

Oxatomide

Signal Name:

DAD1A



## MSD Apex Spectra

RT:

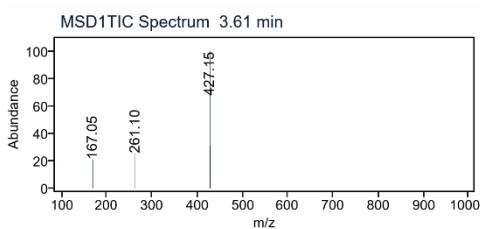
3.610

Sample Name:

Oxatomide

Signal Name:

MSD1TIC



## Biological activity

**Oxatomide**  
**PXR - EC<sub>50</sub> 6 ± 3 μM**  
**2.3 ± 0.3 fold activation**

