

Cilofexor

CAS Registry No.: 1418274-28-8

Formal Name: 2-(3-(2-chloro-4-((5-cyclopropyl-3-(2,6-dichlorophenyl)isoxazol-4-yl)methoxy)phenyl)-3-hydroxyazetid-1-yl)isonicotinic acid

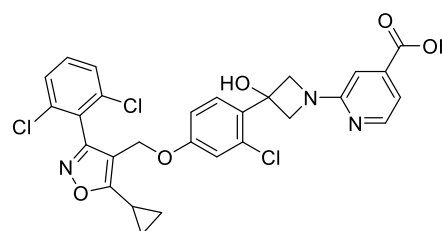
EUBOPEN ID: EUB0001168a

Molecular Formula: C₂₈H₂₂Cl₃N₃O₅

Molecular Weight: 586.85 g/mol

Smiles:
OC(C1=CC=NC(N2CC(O)(C2)C3=C(C=C(C=C3)OCC4=C(ON=C4C5=C(C=CC=C5Cl)Cl)C6CC6)Cl)=C1)=O

Recommended concentration: 1 μM

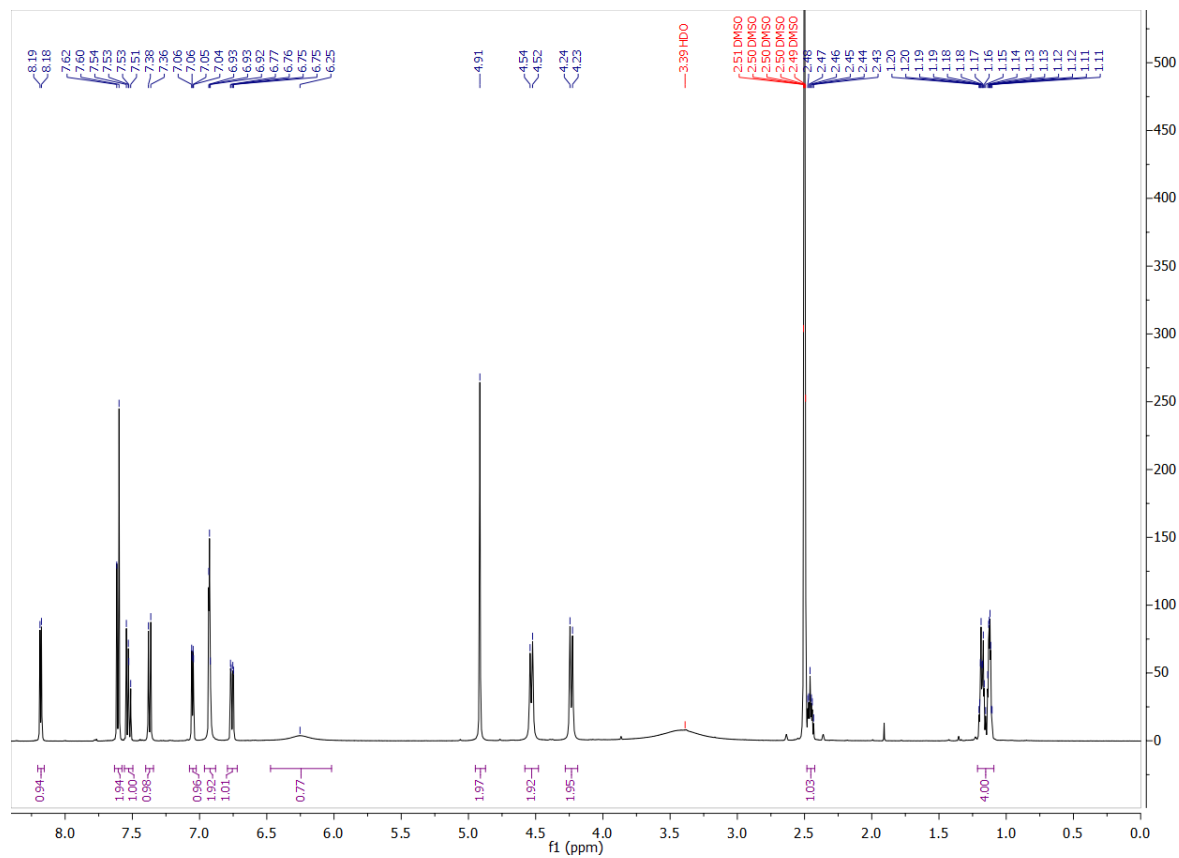


Biological activity

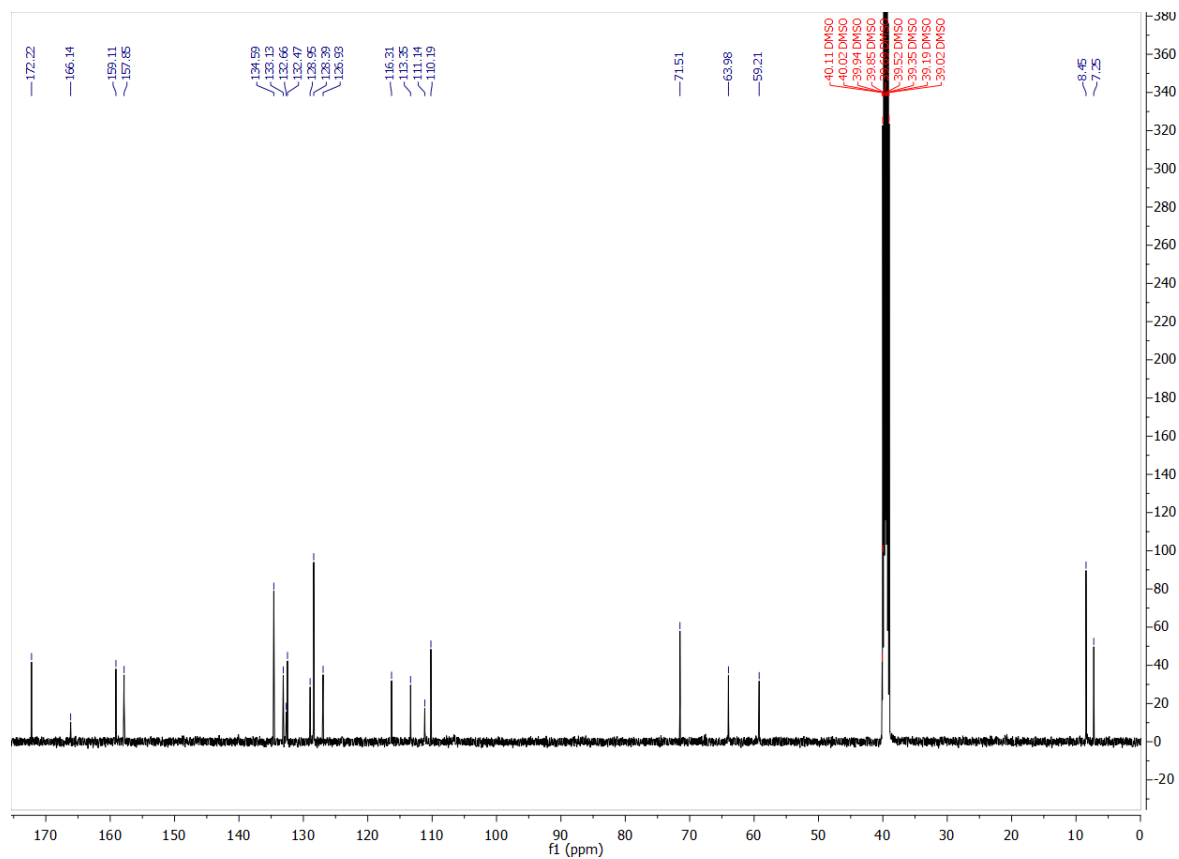
		Type	IC ₅₀ /EC ₅₀ [μM]	Reference
Main NR target:	NR1H4 (FXR)	Agonist	0.04	https://doi.org/10.1021/acs.jmedchem.9b01701
NR off-target:				

Identity

¹H NMR



¹³C NMR



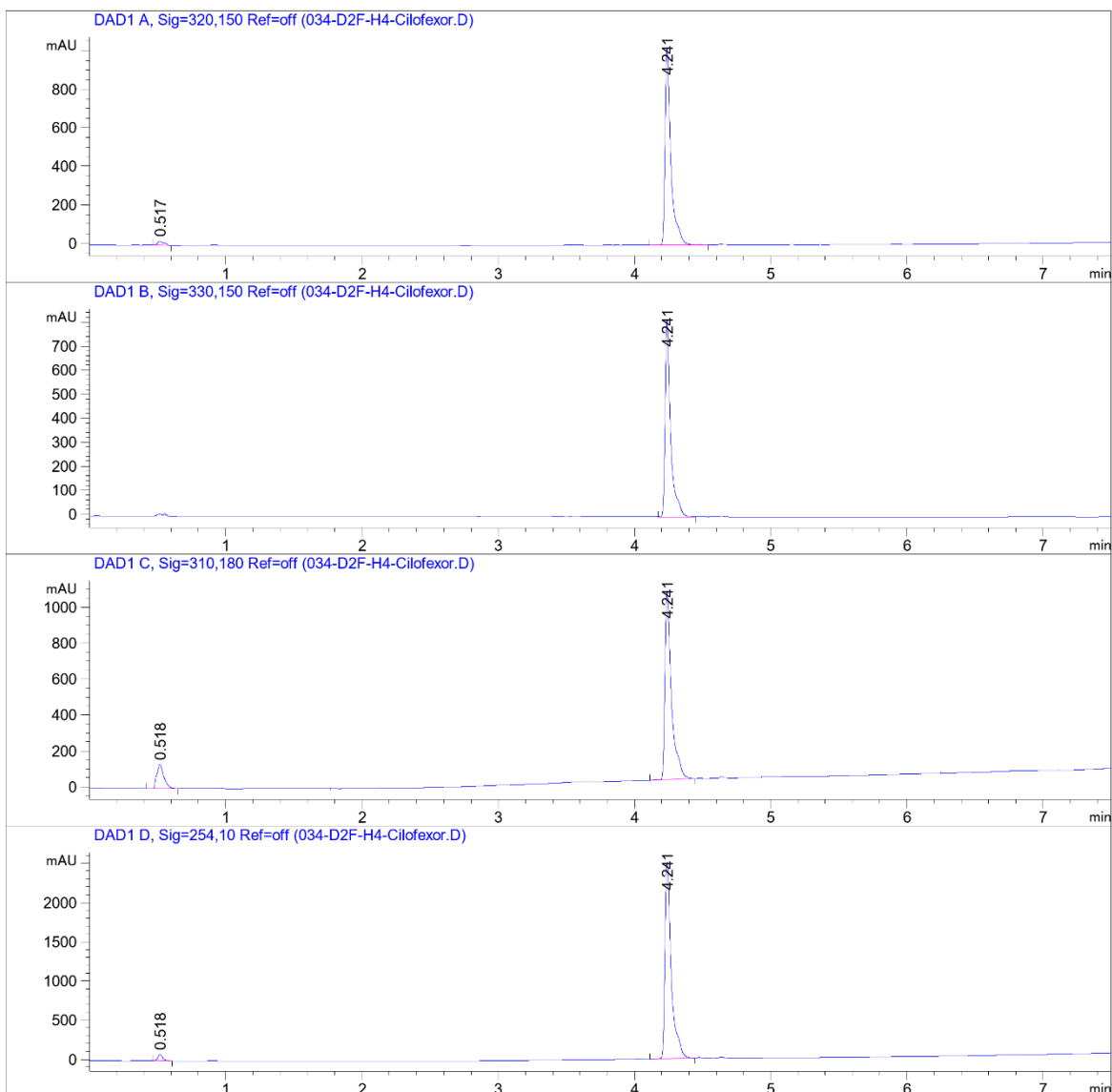
COMPOUND INFORMATION

Purity

Data File W:\analyti...\N\CGC_wave3_1_SecondPass 2023-01-19 20-16-18\034-D2F-H4-Cilofexor.D

Sample Name: Cilofexor

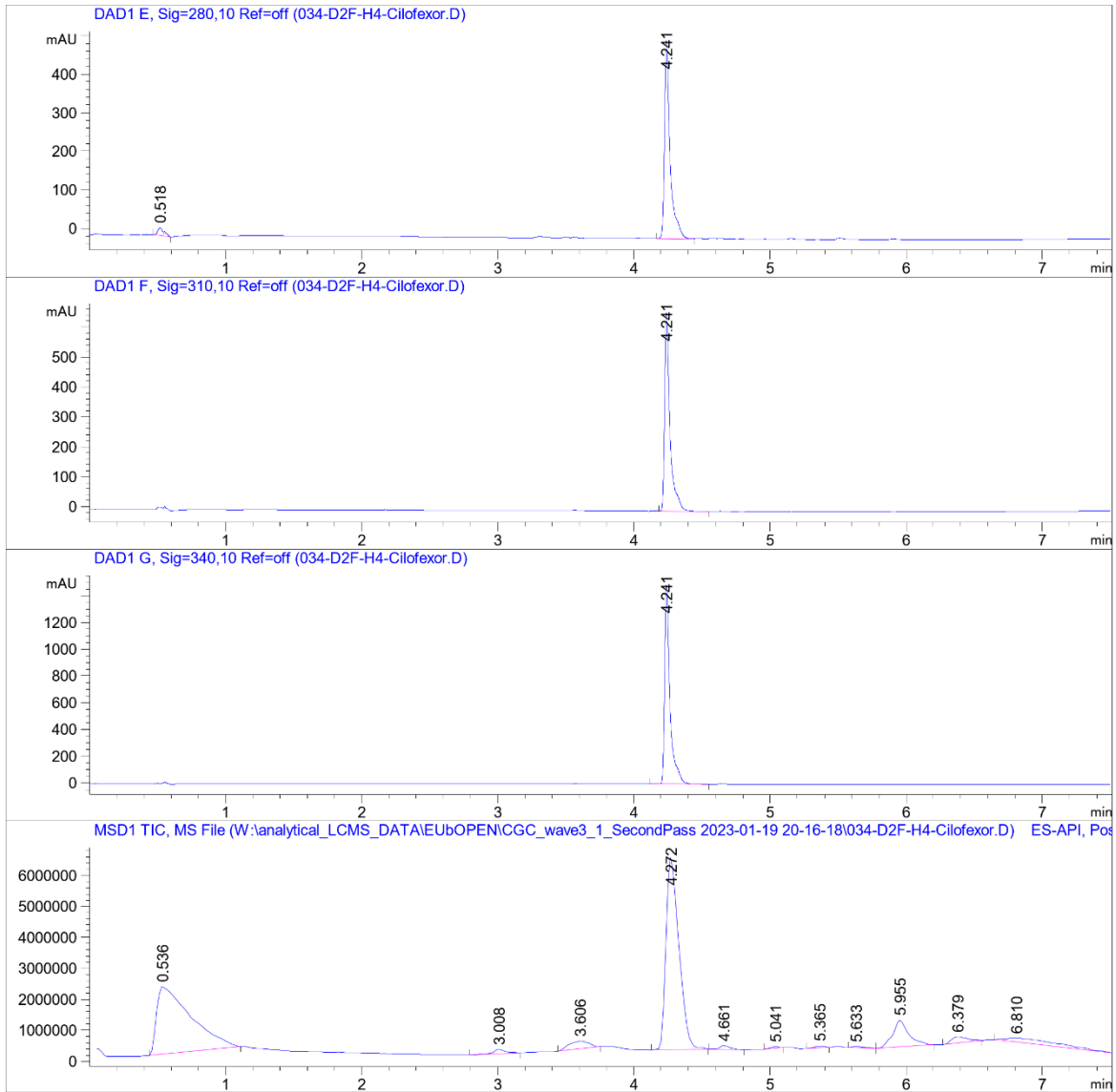
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=====
Acq. Operator   : SYSTEM                      Seq. Line :   34
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2F-H4
Injection Date  : 1/20/2023 2:30:23 AM        Inj       :    1
                                           Inj Volume: Inj prog
Sequence File   : W:\analytical_LCMS_DATA\EUBOPEN\CGC_wave3_1_SecondPass 2023-01-19 20-16-18
                  \CGC_wave3_1_SecondPass.S
Method          : W:\analytical_LCMS_DATA\EUBOPEN\CGC_wave3_1_SecondPass 2023-01-19 20-16-18
                  \CGL_SECONDPASS_NONPOLCOMP_VIAL2+4_20210323.M (Sequence Method)
Last changed    : 7/18/2022 10:07:35 AM by SYSTEM
Method Info     : CGL wellplate, 0.5 uL of 10 mM DMSO. Dilution with MeCN only (9+9 uL)
=====
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COMPOUND INFORMATION

Data File W:\analyti...N\CGC_wave3_1_SecondPass 2023-01-19 20-16-18\034-D2F-H4-Cilofexor.D

Sample Name: Cilofexor



COMPOUND INFORMATION

Data File W:\analyti...\CGC_wave3_1_SecondPass 2023-01-19 20-16-18\034-D2F-H4-Cilofexor.D

Sample Name: Cilofexor

MS Signal: MSD1 TIC, MS File, ES-API, Pos, Scan, Frag: 70, "POS Scan"

Spectra from peak tops.

Noise Cutoff: 1000 counts.

Reportable Ion Abundance: > 50%.

LC Signal: DAD1 A, Sig=320,150 Ref=off

Peak matching window: 0.1 min

Retention Time (LC)	LC Area	Retention Time (MS)	MS Area	Mol. Weight or Ion
0.517	77	0.536	37654432	157.00 I
-	-	3.008	860643	239.00 I 217.00 I
-	-	3.606	2444670	234.00 I 170.80 I
4.241	3045	4.272	40616108	588.10 I 586.10 I
-	-	4.661	609146	602.10 I 600.10 I
-	-	5.041	195912	318.20 I 296.20 I
-	-	5.365	301437	348.20 I 280.20 I 228.20 I 137.10 I
-	-	5.633	316641	507.30 I 280.20 I 137.10 I
-	-	5.955	7029393	282.20 I
-	-	6.379	1609329	400.30 I 284.20 I 282.20 I 137.10 I
-	-	6.810	4163593	282.20 I 137.10 I

