

Tropifexor

CAS Registry No.: 1383816-29-2

Formal Name: 2-(3-((5-cyclopropyl-3-(2-(trifluoromethoxy)phenyl)isoxazol-4-yl)methoxy)-8-azabicyclo[3.2.1]octan-8-yl)-4-fluorobenzo[d]thiazole-6-carboxylic acid

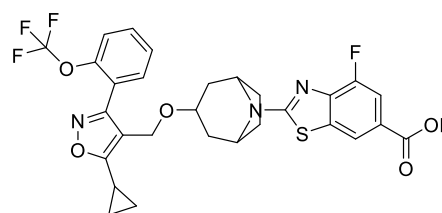
EUBOPEN ID: EUB0001169a

Molecular Formula: C₂₉H₂₅F₄N₃O₅S

Molecular Weight: 603.59 g/mol

Smiles:
O=C(C1=CC(F)=C2N=C(N3C4CC(OCC5=C(C6CC6)ON=C5C7=CC=C(C=C7)OC(F)(F)F)CC3CC4)SC2=C1)O

Recommended concentration: 1 μM

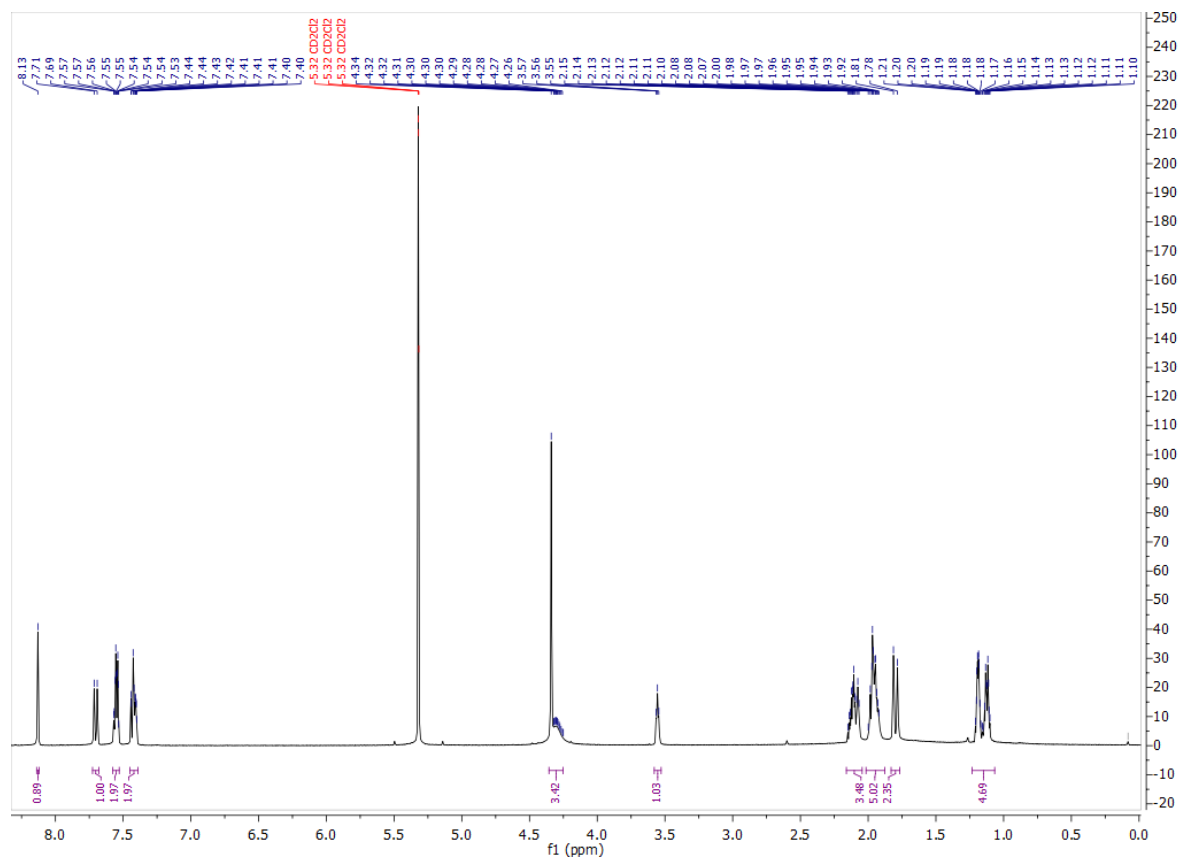


Biological activity

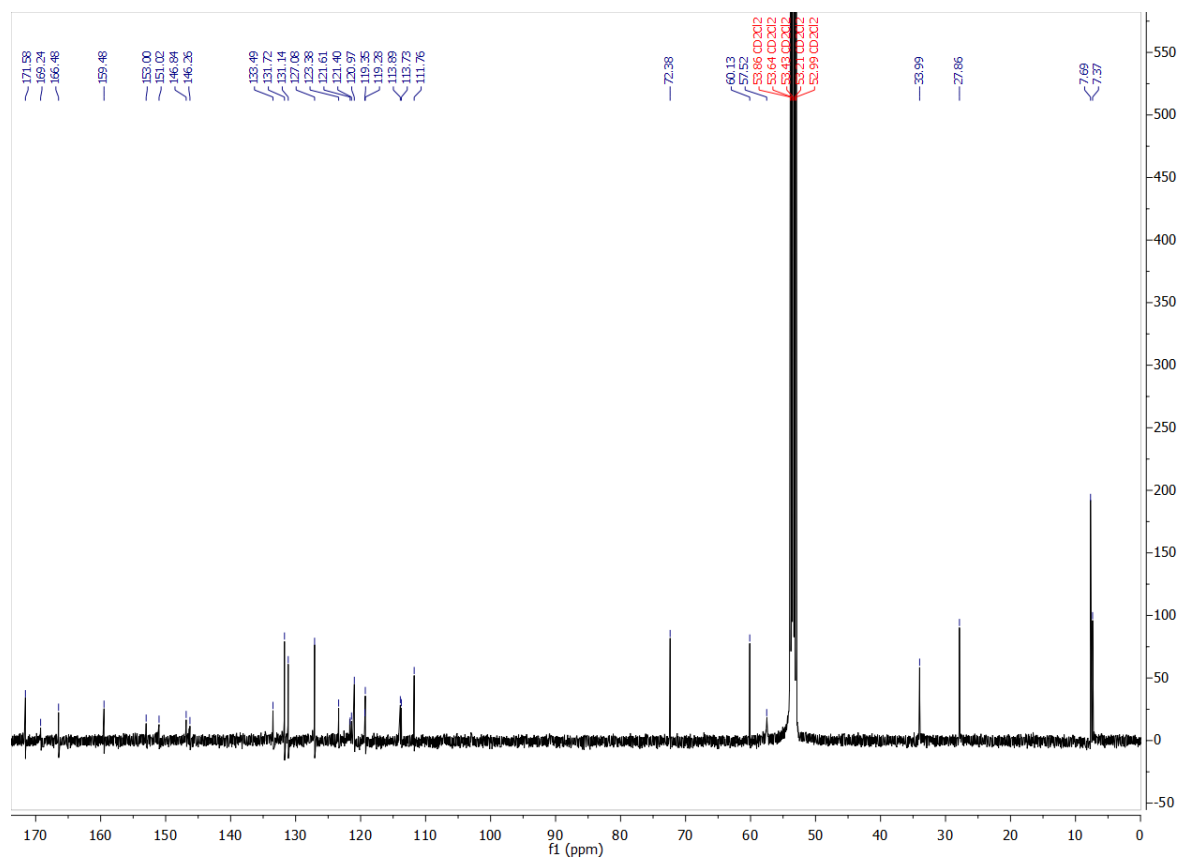
		Type	IC ₅₀ /EC ₅₀ [μM]	Reference
Main NR target:	NR1H4 (FXR)	Agonist	0.0003	https://doi.org/10.1021/acs.jmedchem.7b00907
NR off-target:				

Identity

¹H NMR



¹³C NMR



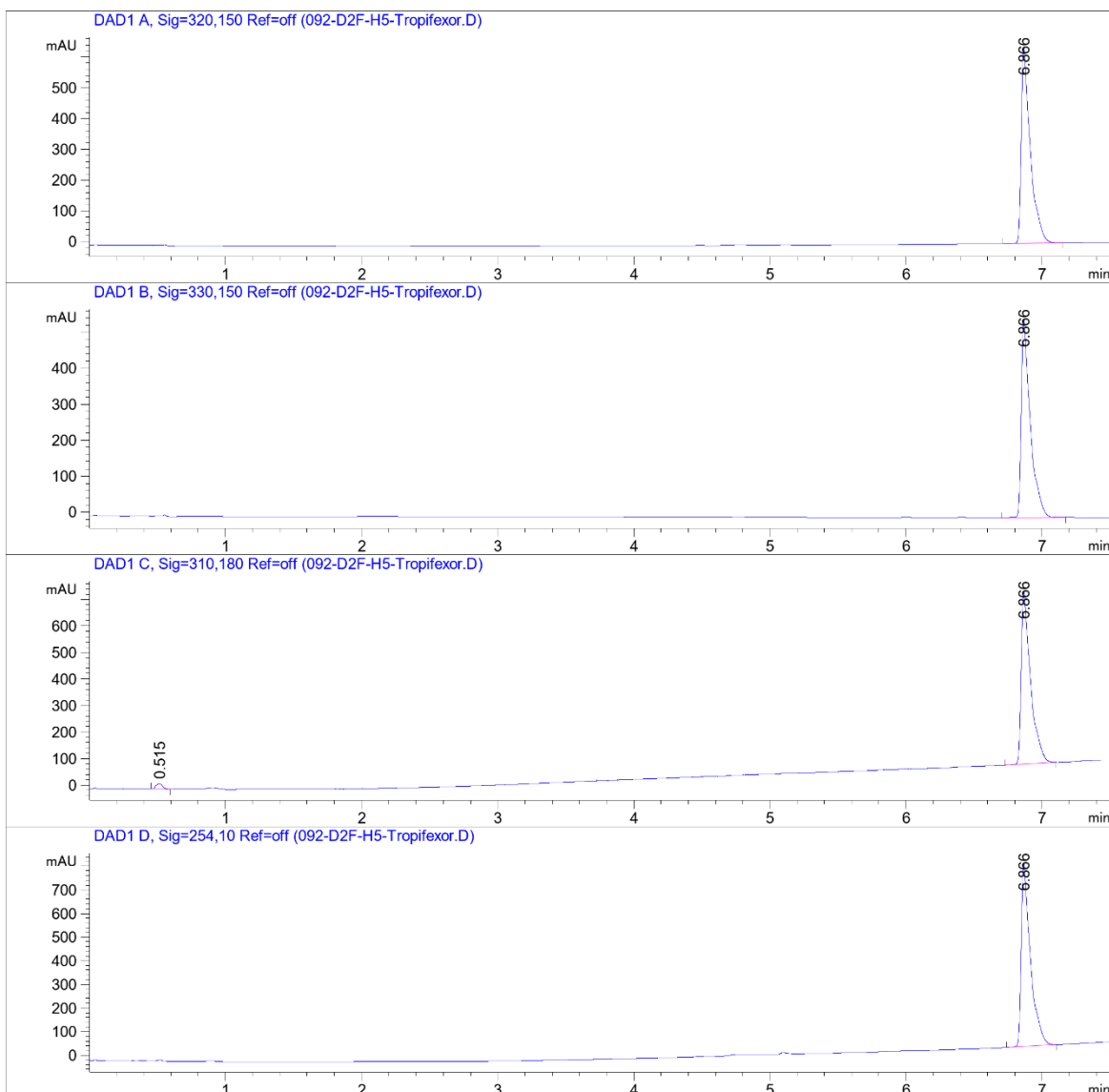
COMPOUND INFORMATION

Purity

Data File W:\analyti...\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\092-D2F-H5-Tropifexor.D

Sample Name: Tropifexor

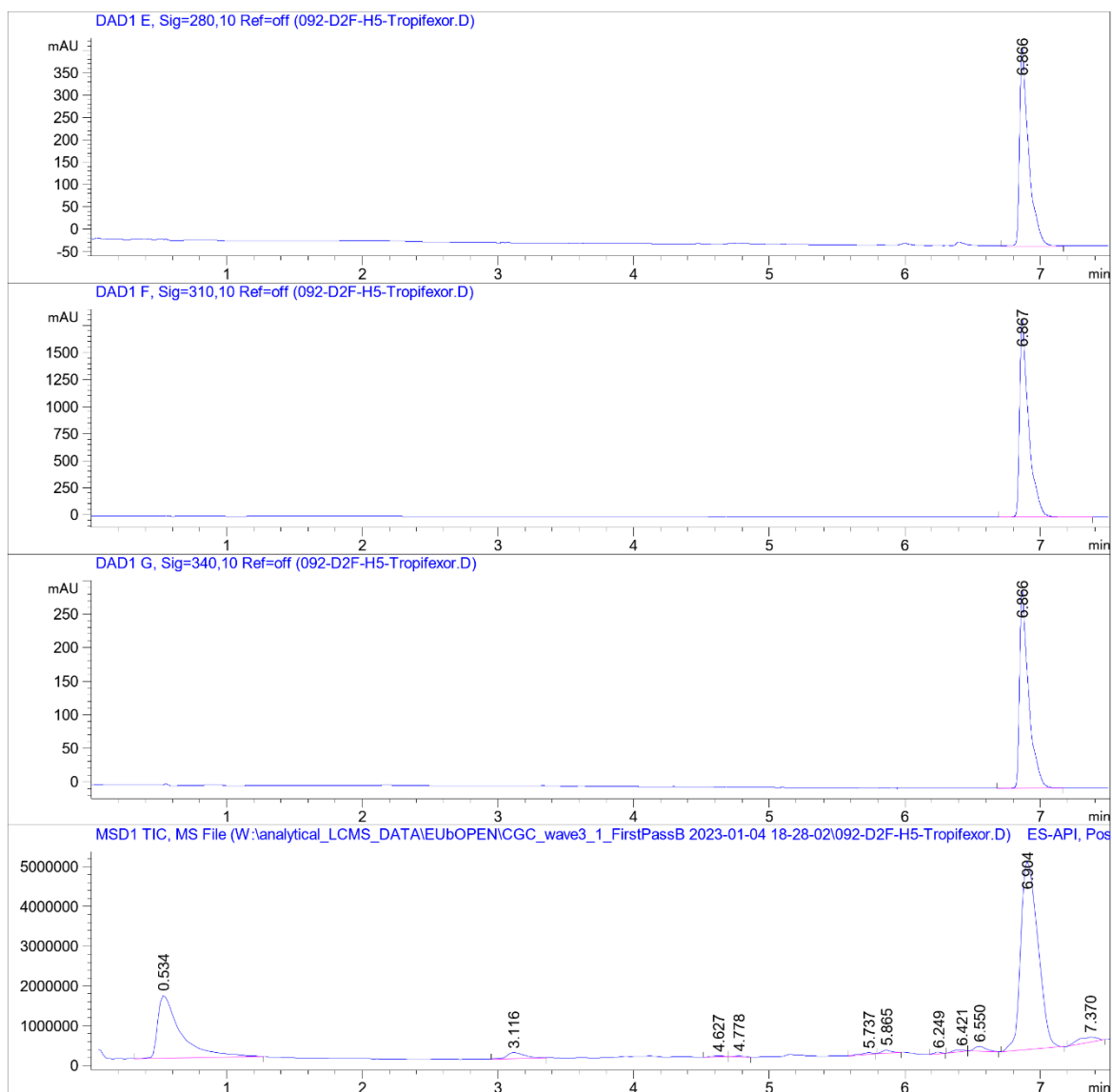
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=====
Acq. Operator   : SYSTEM                      Seq. Line :   92
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2F-H5
Injection Date  : 1/5/2023 11:17:09 AM       Inj       :    1
                                           Inj Volume: Inj prog
Sequence File   : W:\analytical_LCMS_DATA\EUBOPEN\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02
                  \CGC_wave3_1_FirstPassB.S
Method          : W:\analytical_LCMS_DATA\EUBOPEN\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02
                  \CGL_FIRSTPASS_GENERALMETHOD_VIAL1+2_20210319.M (Sequence Method)
Last changed    : 1/25/2022 4:36:18 PM by SYSTEM
Method Info     : CGL wellplate, 0.5 uL of 10 mM DMSO, general method
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COMPOUND INFORMATION

Data File W:\analyti...\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\092-D2F-H5-Tropifexor.D

Sample Name: Tropifexor



COMPOUND INFORMATION



Data File W:\analyti...\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\092-D2F-H5-Tropifexor.D

Sample Name: Tropifexor

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
-	-	0.534	18485472	157.00 I
-	-	3.116	1355728	239.00 I 217.10 I
-	-	4.627	161282	510.30 I 170.90 I 158.20 I 137.10 I
-	-	4.778	134497	279.10 I 137.10 I
-	-	5.737	206667	280.20 I
-	-	5.865	370628	318.20 I 296.20 I
-	-	6.249	167731	228.20 I 137.10 I
-	-	6.421	234804	350.20 I 282.20 I 254.20 I 137.10 I
-	-	6.550	724366	507.30 I 485.30 I 280.20 I
6.866	2926	6.904	41956712	604.20 I
-	-	7.370	1335602	400.30 I 282.20 I

