

Lanifibranor

CAS Registry No.: 927961-18-0

Formal Name: 4-(1-(benzo[d]thiazol-6-ylsulfonyl)-5-chloro-1H-indol-2-yl)butanoic acid

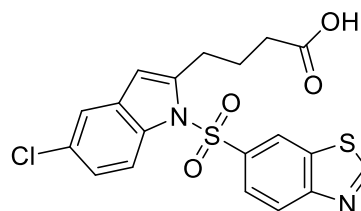
EUbOPEN ID: EUB0001149a

Molecular Formula: C₁₉H₁₅ClN₂O₄S₂

Molecular Weight: 434.91 g/mol

Smiles: C1=CC2=C(C=C1S(=O)(=O)N3C4=C(C=C(C=C4)Cl)C=C3CCCC(=O)O)SC=N2

Recommended concentration: 1 μM

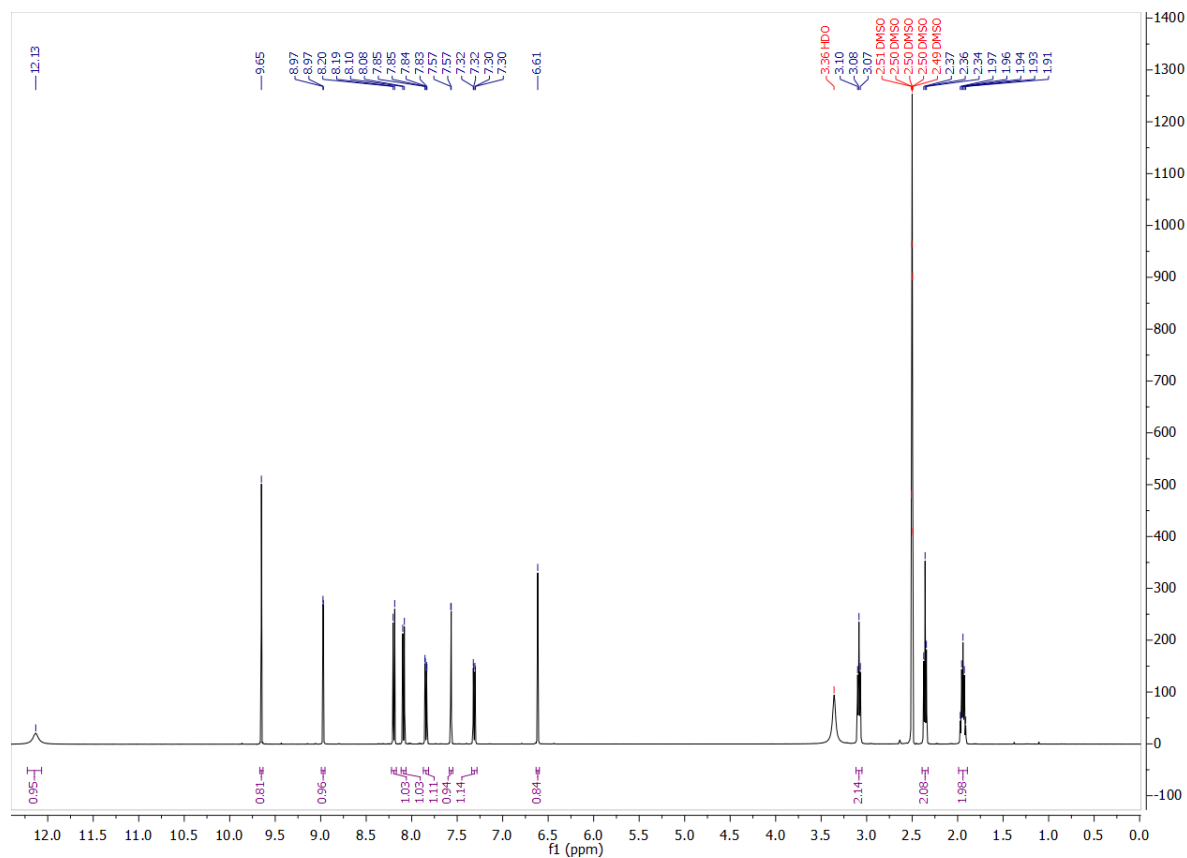


Biological activity

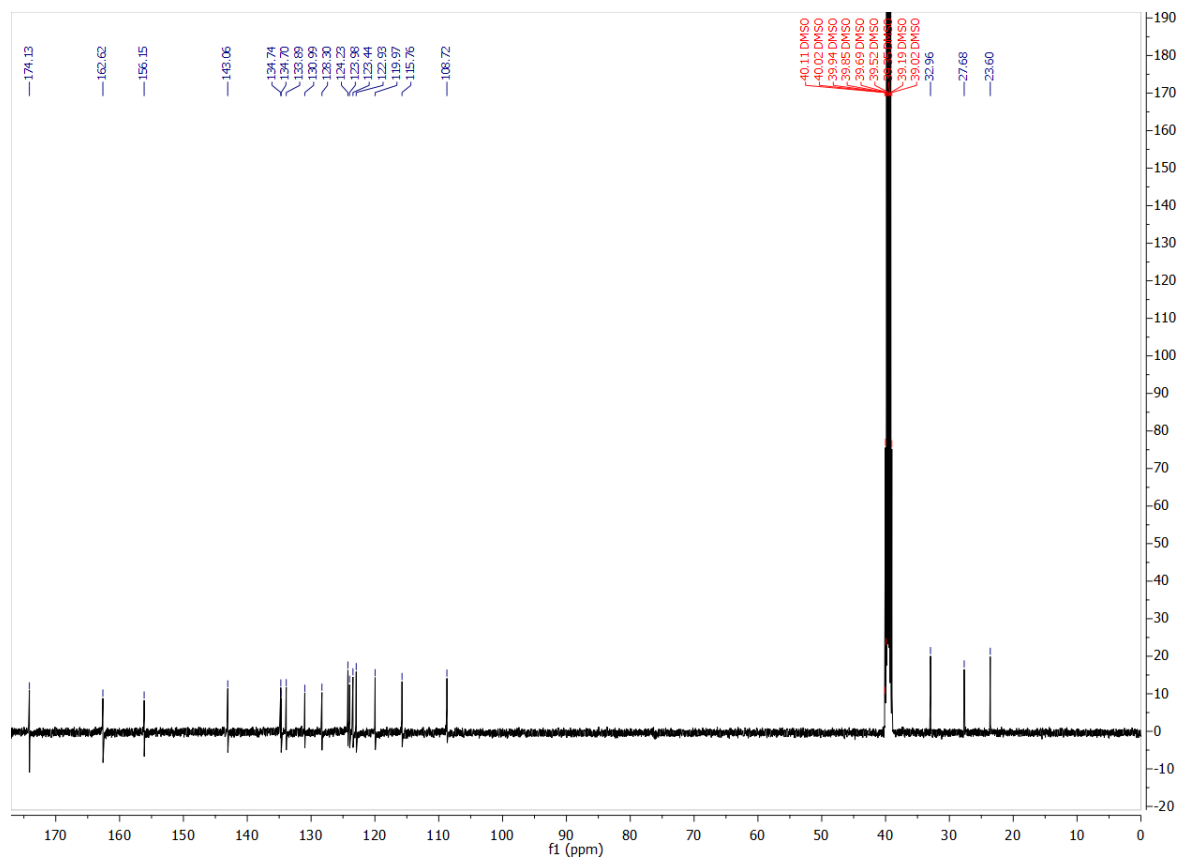
		Type	IC ₅₀ /EC ₅₀ [μM]	Reference
Main NR target:	NR1C2 (PPARδ)	Agonist	0.9	https://doi.org/10.1021/acs.jmedchem.7b01285
	NR1C3 (PPARγ)	Agonist	0.21	
NR off-target:	NR1C1 (PPARα)	Agonist	1.5.	https://doi.org/10.1021/acs.jmedchem.7b01285

Identity

¹H NMR



¹³C NMR



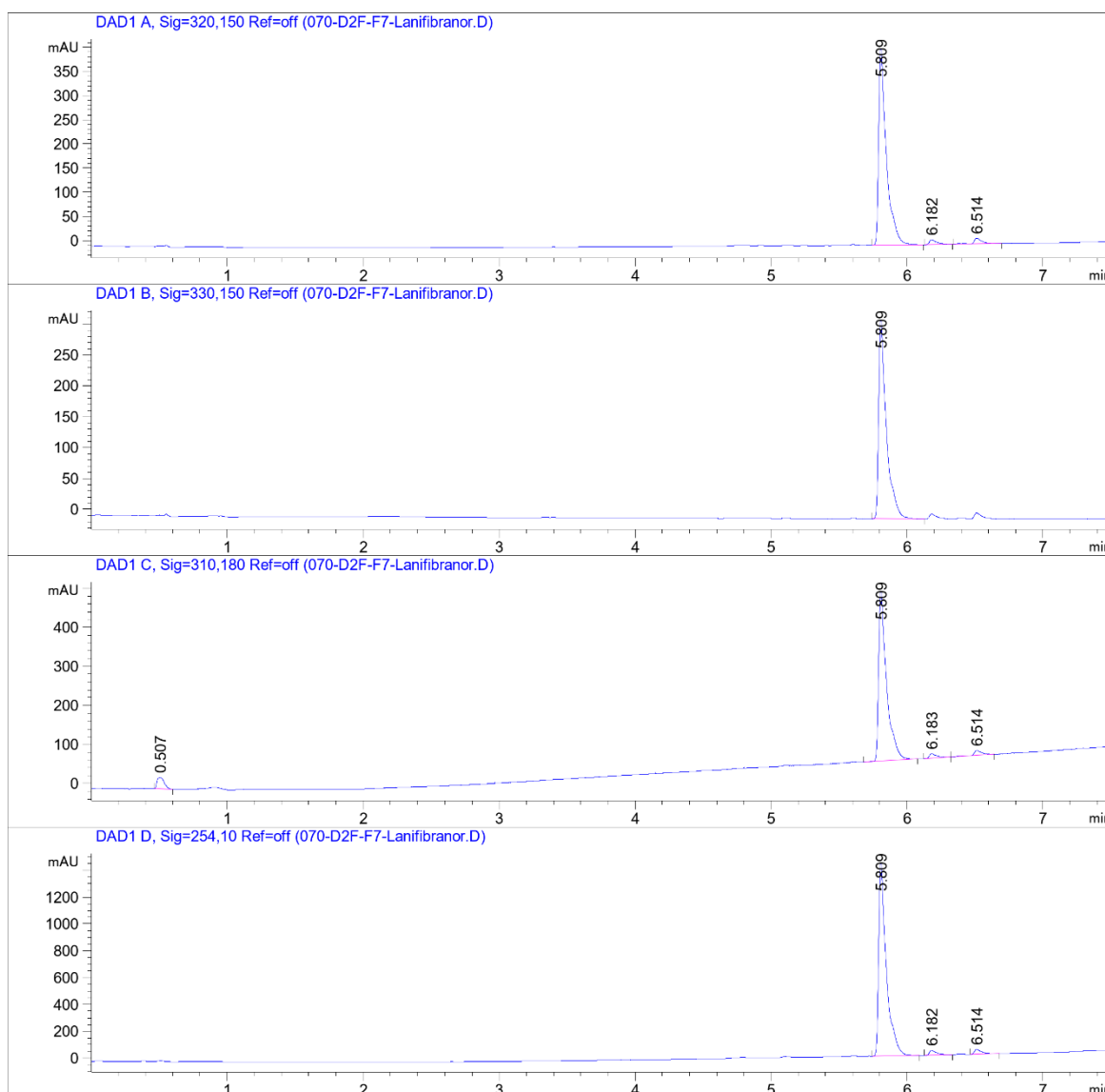
COMPOUND INFORMATION

Purity

Data File W:\analyti...GC_wave3_1_FirstPassB 2023-01-04 18-28-02\070-D2F-F7-Lanifibranor.D

Sample Name: Lanifibranor

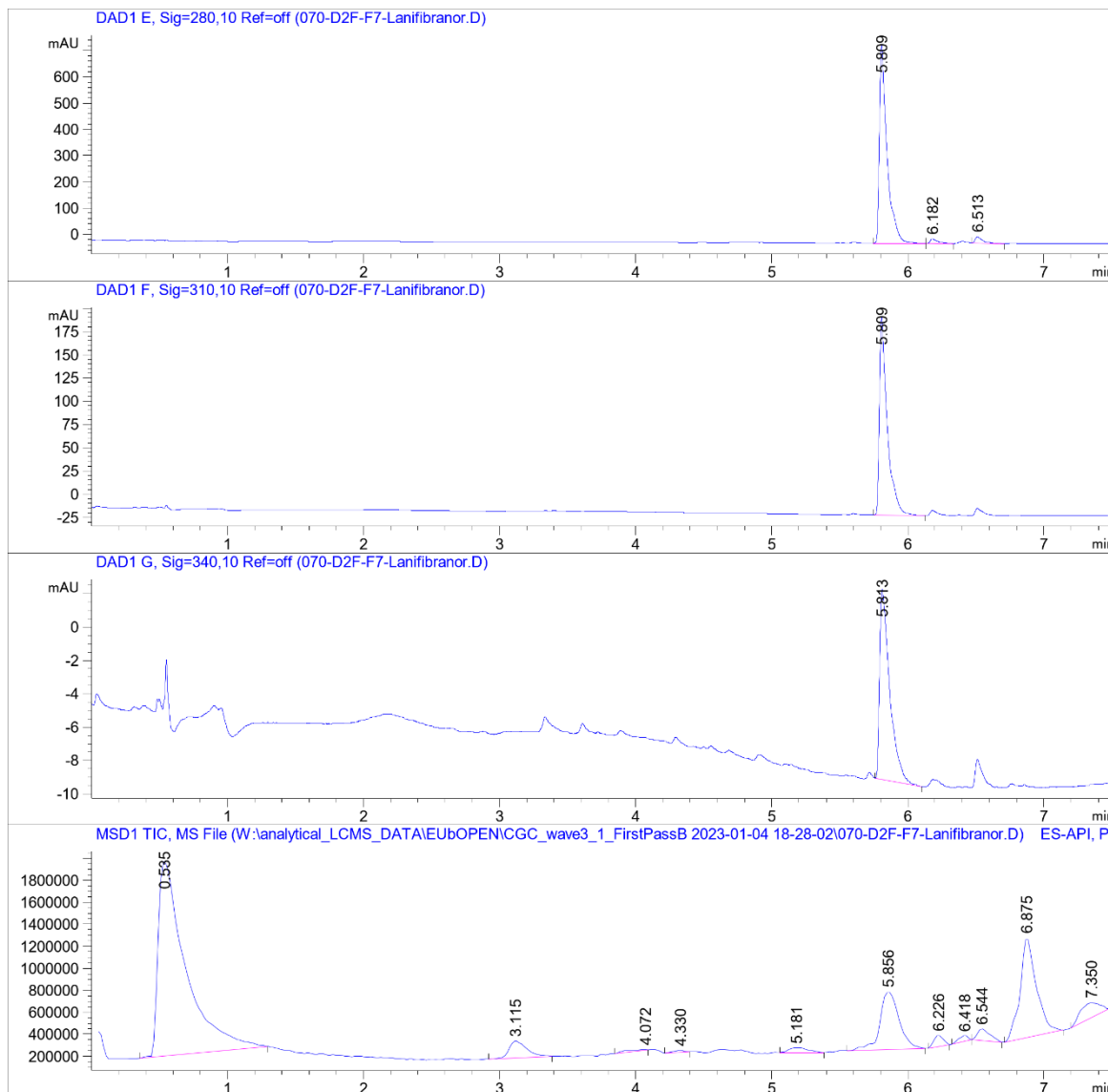
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=====
Acq. Operator   : SYSTEM                      Seq. Line :   70
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2F-F7
Injection Date  : 1/5/2023 7:13:50 AM        Inj       :    1
                                           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...GC_wave3_1_FirstPassB 2023-01-04 18-28-02\070-D2F-F7-Lanifibranor.D

Sample Name: Lanifibranor



COMPOUND INFORMATION

Data File W:\analyti...GC_wave3_1_FirstPassB 2023-01-04 18-28-02\070-D2F-F7-Lanifibranor.D

Sample Name: Lanifibranor

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
-	-	0.535	24951508	157.00 I
-	-	3.115	1434967	239.00 I 217.00 I
-	-	4.072	151780	170.90 I
-	-	4.330	99141	510.40 I 170.80 I
-	-	5.181	436414	510.40 I 170.90 I 137.10 I
5.809	1583	5.856	5196727	435.00 I
6.182	40	6.226	496043	449.00 I 228.20 I 137.10 I
-	-	6.418	222562	282.20 I 254.20 I
6.514	58	6.544	668935	507.20 I 280.20 I
-	-	6.875	7607204	282.30 I
-	-	7.350	1427781	400.30 I 282.20 I

