

GSK3787

CAS Registry No.: 188591-46-0

Formal Name: 4-chloro-N-(2-((5-(trifluoromethyl)pyridin-2-yl)sulfonyl)ethyl)benzamide

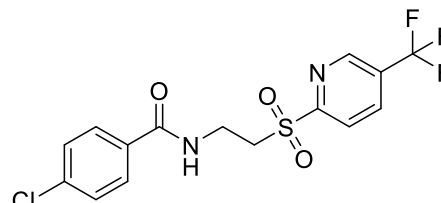
EUBOPEN ID: EUB0001151a

Molecular Formula: C₁₅H₁₂ClF₃N₂O₃S

Molecular Weight: 392.78 g/mol

Smiles: C1=CC(=CC=C1C(=O)NCCS(=O)(=O)C2=NC=C(C=C2)C(F)(F)F)Cl

Recommended concentration: 1 μM

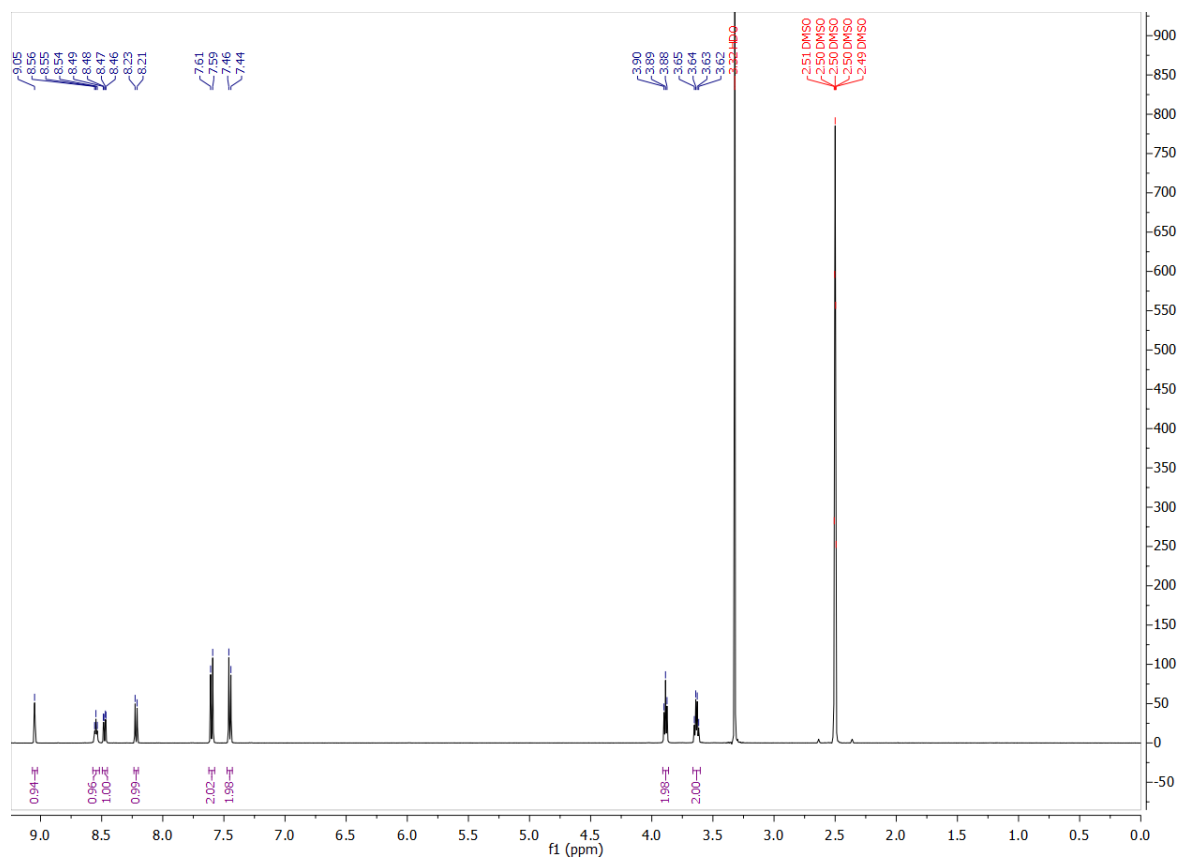


Biological activity

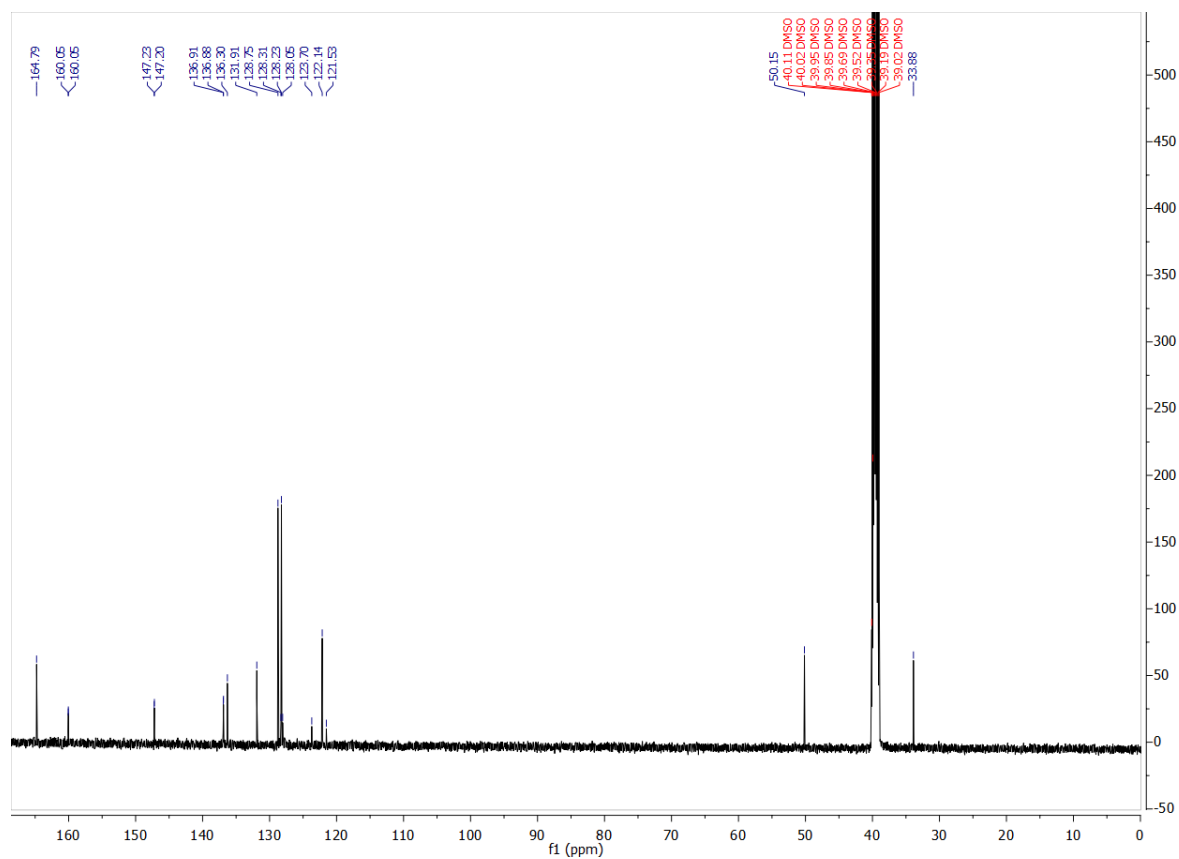
		Type	IC ₅₀ /EC ₅₀ [μM]	Reference
Main NR target:	NR1C2 (PPARδ)	Antagonist	0.13	https://doi.org/10.1021/jm900464j
NR off-target:	NR1C3 (PPARγ)	Antagonist	5	inhouse

Identity

¹H NMR



¹³C NMR



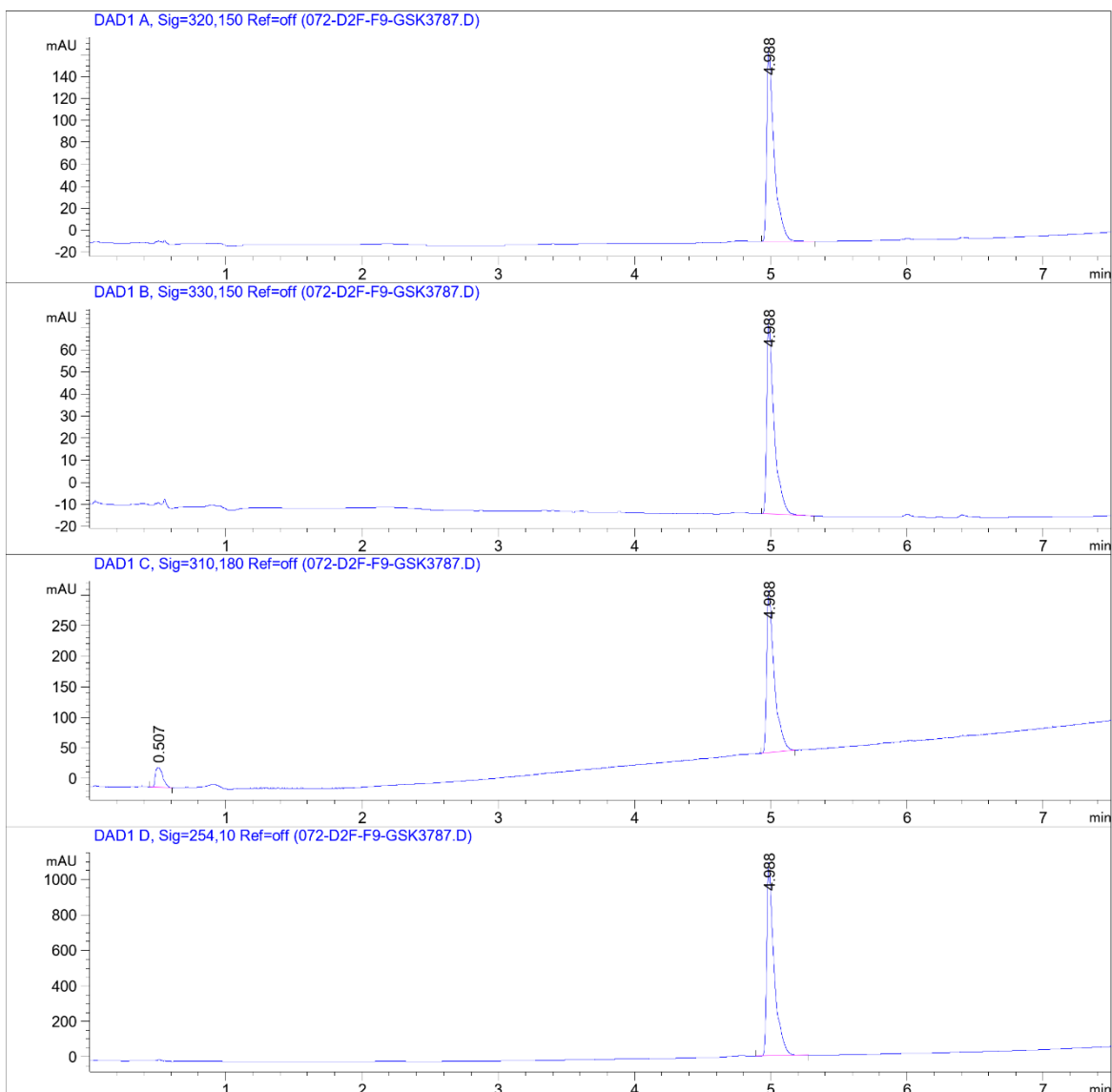
COMPOUND INFORMATION

Purity

Data File W:\analyti...PEN\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\072-D2F-F9-GSK3787.D

Sample Name: GSK3787

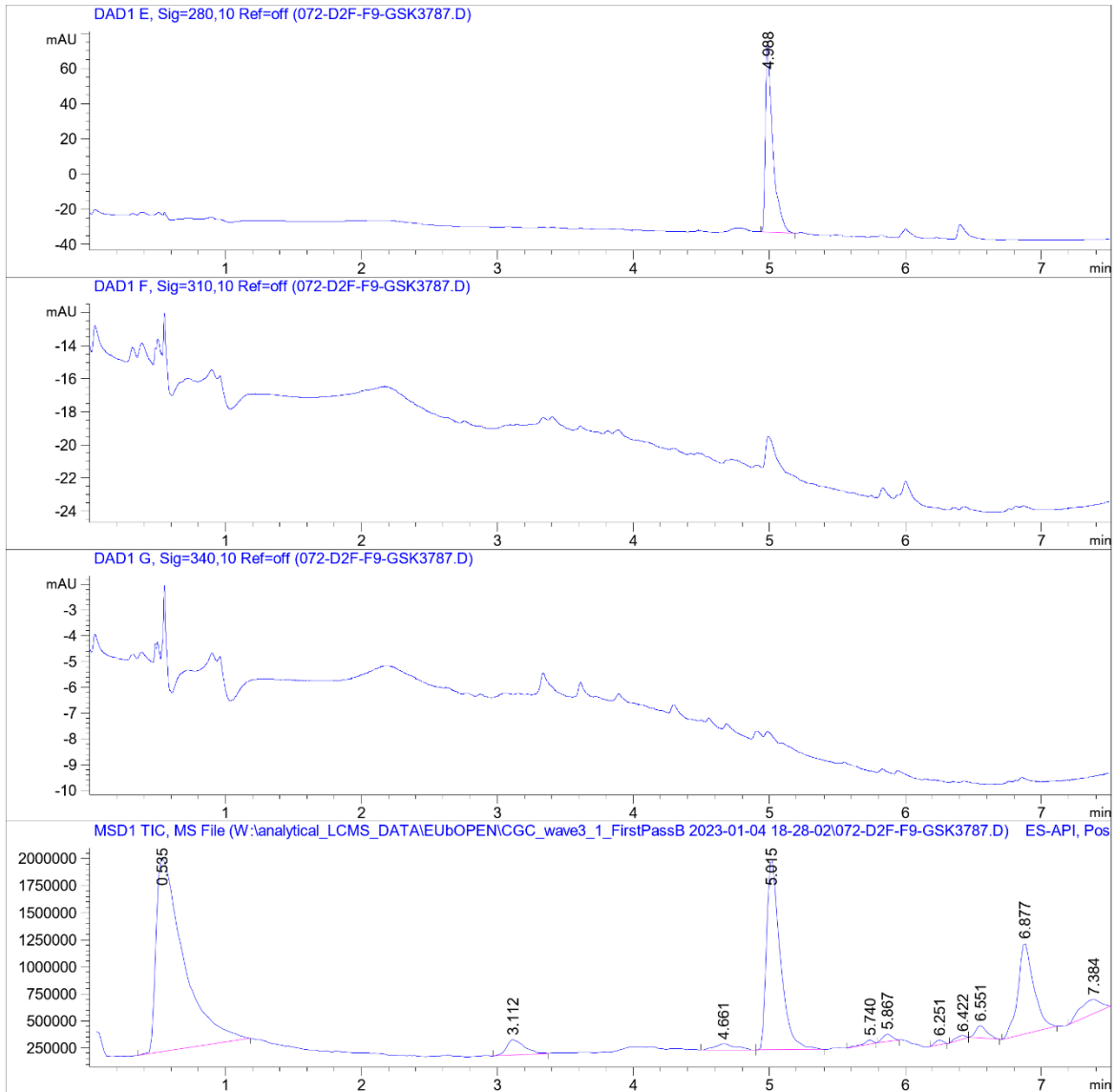
```
=====
Acq. Operator   : SYSTEM                      Seq. Line :   72
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2F-F9
Injection Date  : 1/5/2023 7:35:56 AM        Inj       :    1
                                           Inj Volume: Inj prog
Sequence File   : 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...PEN\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\072-D2F-F9-GSK3787.D

Sample Name: GSK3787



COMPOUND INFORMATION



Data File W:\analyti...PEN\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\072-D2F-F9-GSK3787.D

Sample Name: GSK3787

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

Spectra from peak tops.

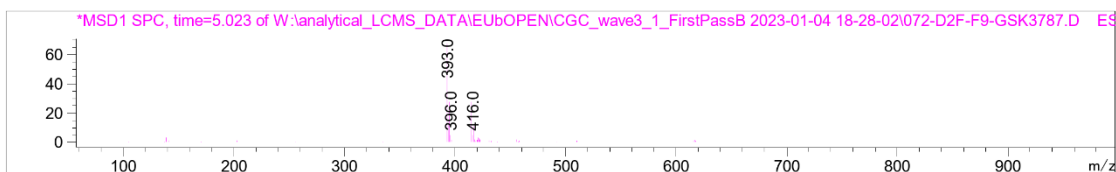
Noise Cutoff: 1000 counts.

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	24993354	157.10 I
-	-	3.112	1282369	239.00 I 217.10 I
-	-	4.661	595512	510.40 I 170.90 I 158.10 I
4.988	657	5.015	12271467	393.00 I
-	-	5.740	177366	280.20 I
-	-	5.867	320988	318.20 I 296.20 I
-	-	6.251	181166	228.20 I 137.10 I
-	-	6.422	175819	350.20 I 282.20 I 254.20 I 137.10 I
-	-	6.551	635696	507.20 I 485.30 I 280.20 I
-	-	6.877	6791576	282.20 I
-	-	7.384	1494212	400.30 I 282.20 I



COMPOUND INFORMATION

Biological activity

GSK3787
PPAR γ - IC₅₀ 5 \pm 1 μ M
0.64 \pm 0.07 rem. activity

