

COMPOUND INFORMATION

SR9009

CAS Registry No.: 1379686-30-2

Formal Name: Ethyl 3-(((4-chlorobenzyl)((5-nitrothiophen-2-yl)methyl)amino)methyl)pyrrolidine-1-carboxylate

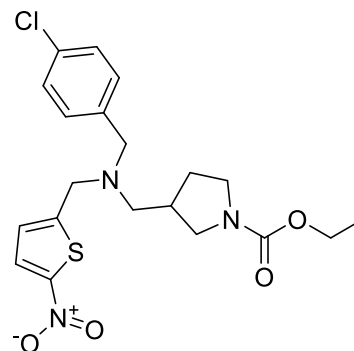
EUBOPEN ID: EUB0001152a

Molecular Formula: C₂₀H₂₄ClN₃O₄S

Molecular Weight: 437.94 g/mol

Smiles: CCOC(=O)N1CCC(C1)CN(CC2=C=C(C=C2)Cl)CC3=CC=C(S3)[N+](=O)[O-]

Recommended concentration: 10 μM



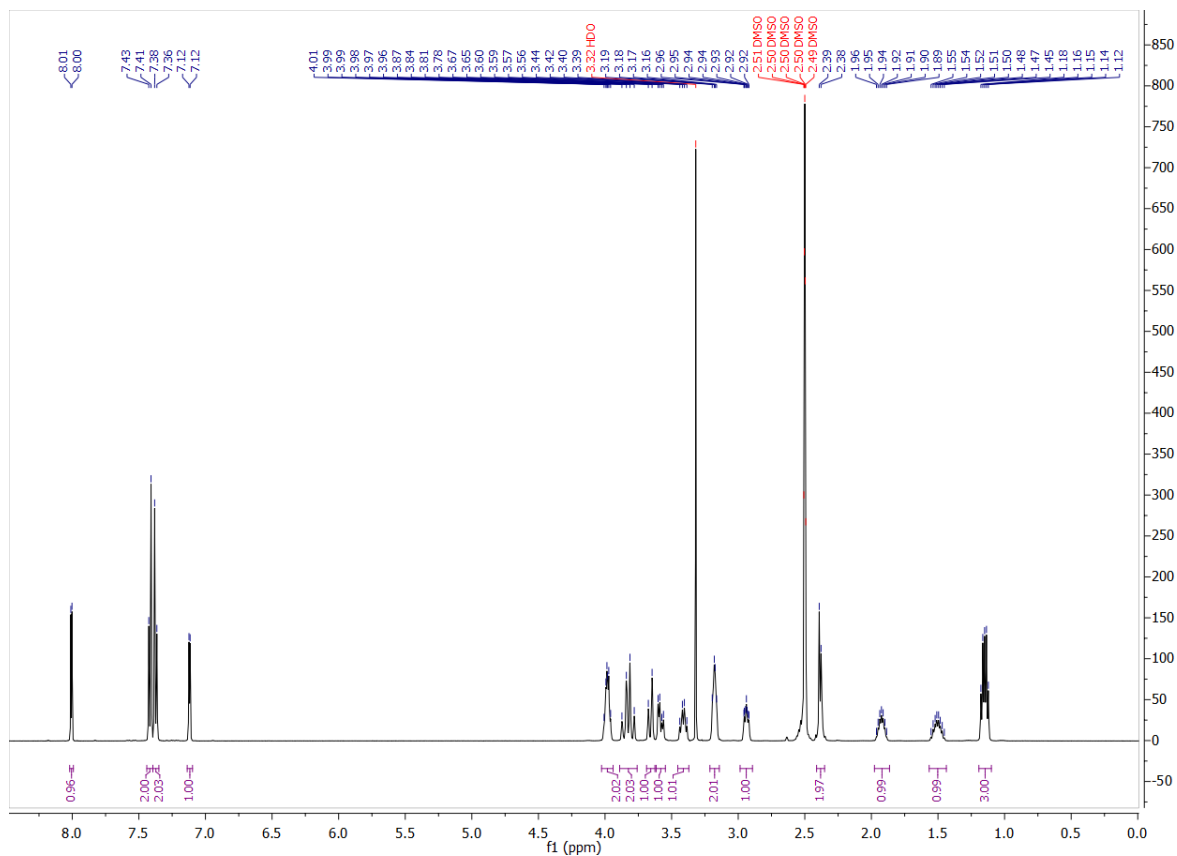
Biological activity

		Type	IC ₅₀ /EC ₅₀ [μM]	Reference
Main NR target:	NR1D1 (revERBα)	Agonist	6.0	inhouse
	NR1D2 (revERBβ)	Agonist	11	
NR off-target:				

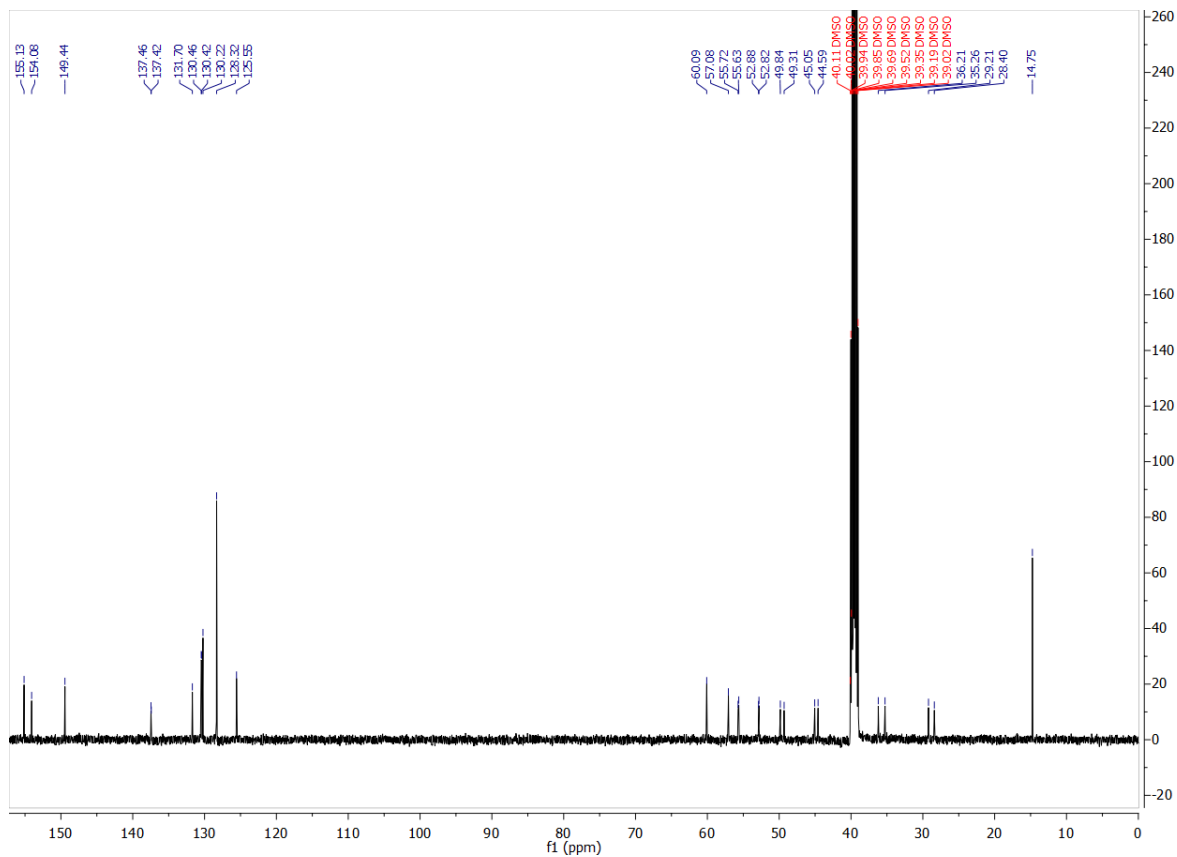
COMPOUND INFORMATION

Identity

¹H NMR



¹³C NMR



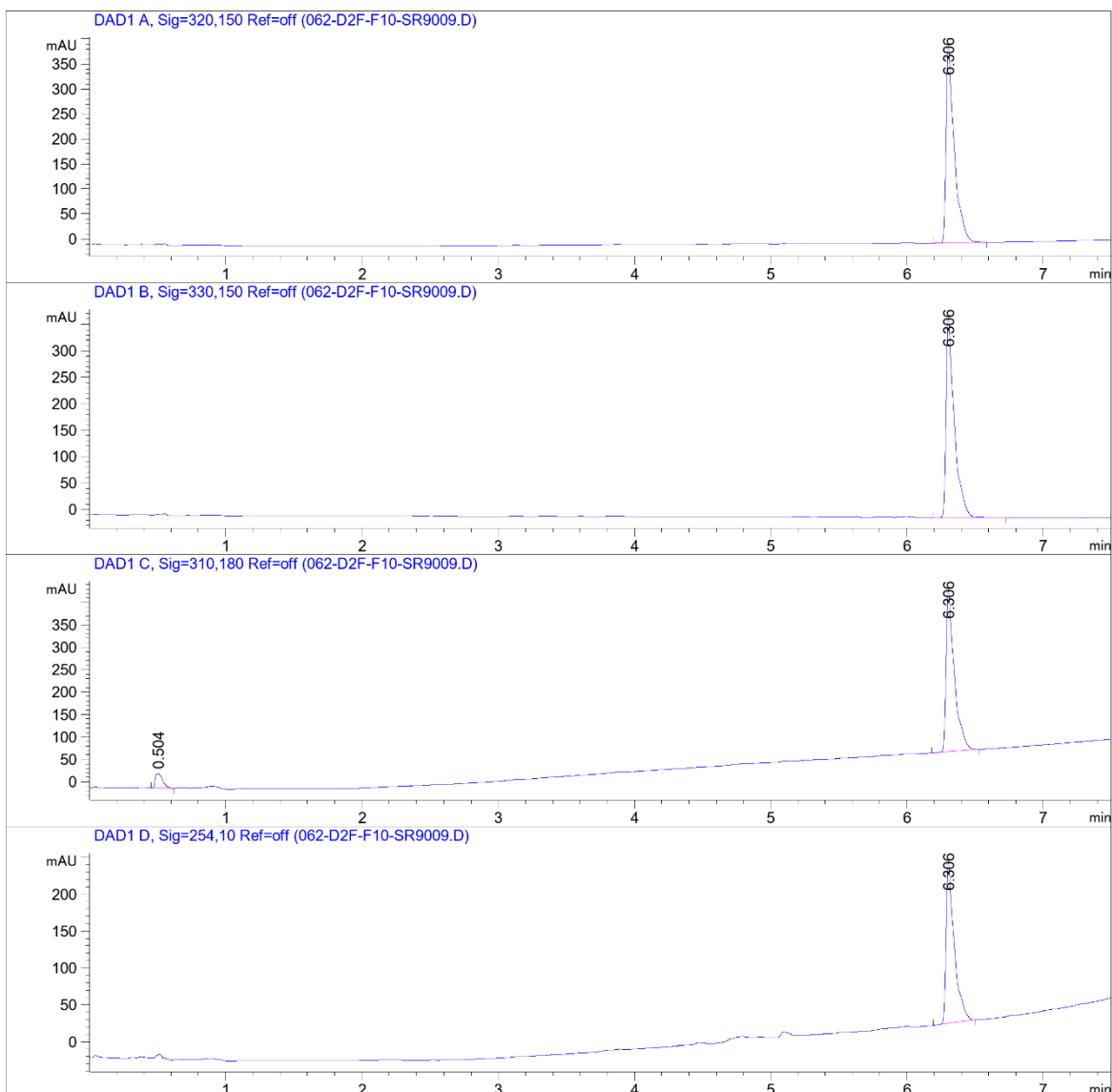
COMPOUND INFORMATION

Purity

Data File W:\analyti...PEN\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\062-D2F-F10-SR9009.D

Sample Name: SR9009

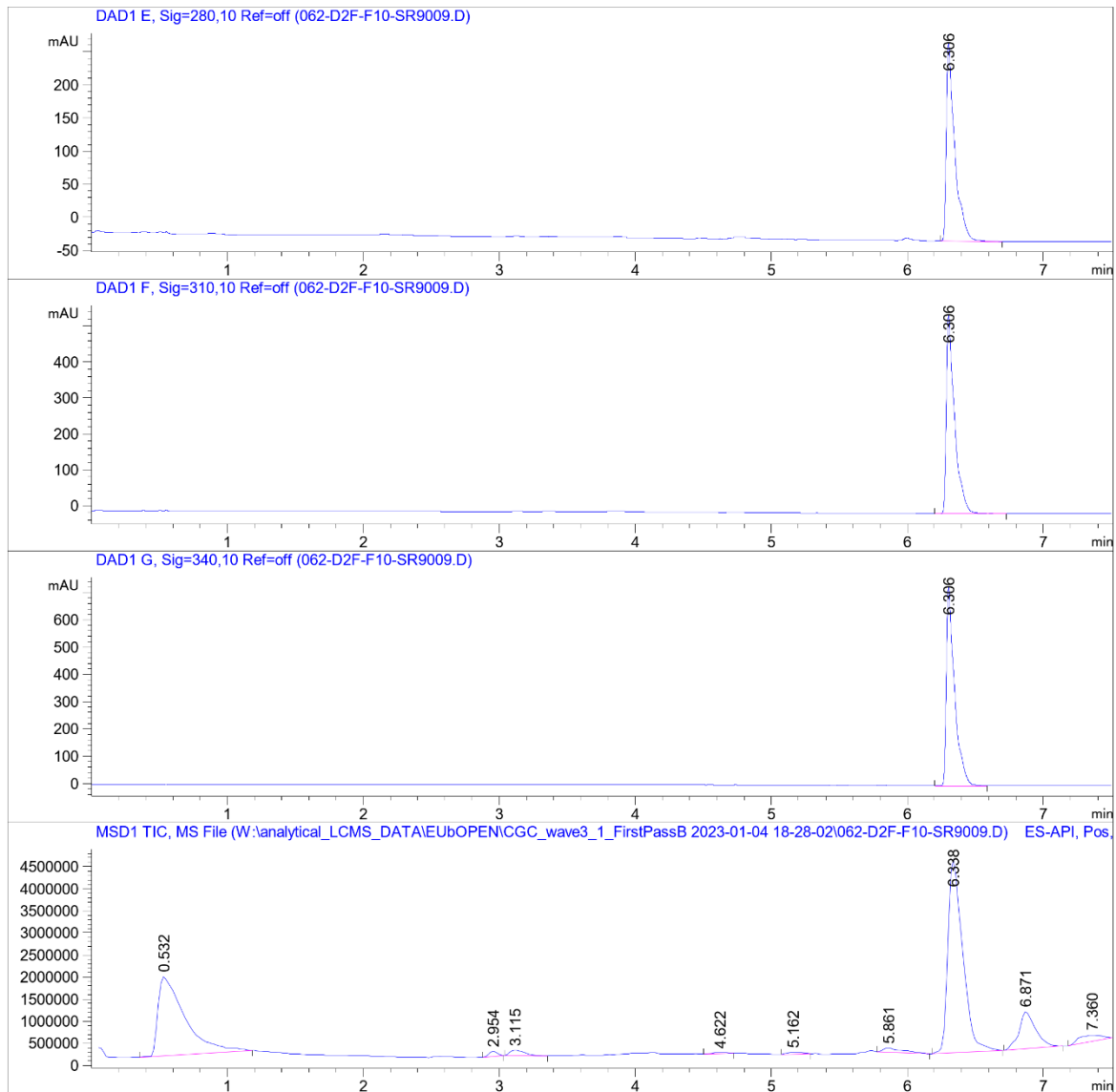
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=====
Acq. Operator   : SYSTEM                      Seq. Line :   62
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2F-F10
Injection Date  : 1/5/2023 5:45:22 AM        Inj       :    1
                                           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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Data File W:\analyti...PEN\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\062-D2F-F10-SR9009.D

Sample Name: SR9009



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Data File W:\analyti...PEN\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\062-D2F-F10-SR9009.D

Sample Name: SR9009

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

Spectra from peak tops.

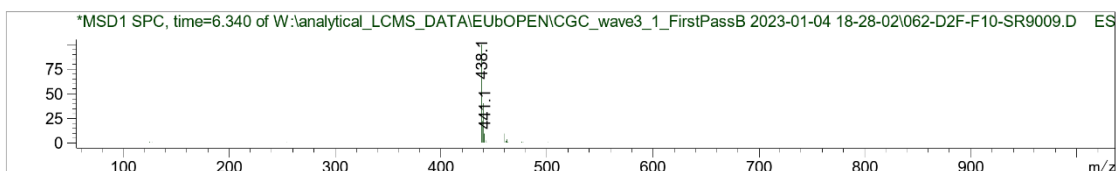
Noise Cutoff: 1000 counts.

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
-	-	0.532	24555990	157.00 I
-	-	2.954	504443	297.10 I
-	-	3.115	951776	239.00 I 217.10 I
-	-	4.622	206301	510.40 I 170.80 I
-	-	5.162	321651	510.40 I 170.90 I 137.20 I
-	-	5.861	886477	318.20 I 296.20 I
6.306	1631	6.338	33107130	438.10 I
-	-	6.871	7148443	282.20 I
-	-	7.360	1752307	400.40 I 282.30 I



Biological activity

