

SR9238

CAS Registry No.: 1416153-62-2

Formal Name: Ethyl 5-(((2,4,6-trimethyl-N-((3'-(methylsulfonyl)-[1,1'-biphenyl]-4-yl)methyl)phenyl)sulfonamido)methyl)furan-2-carboxylate

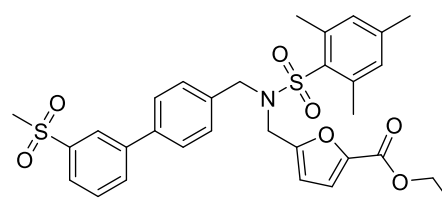
EUBOPEN ID: EUB0000082b

Molecular Formula: C₃₁H₃₃NO₇S₂

Molecular Weight: 595.73 g/mol

Smiles:
CS(C1=CC=CC(C2=CC=C(C=C2)C)N(S(C3=C(C=C(C=C3C)C)C)(=O)=O)CC4=CC=C(O4)C(OCC)=O)=C1)(=O)=O

Recommended concentration: 1 μM

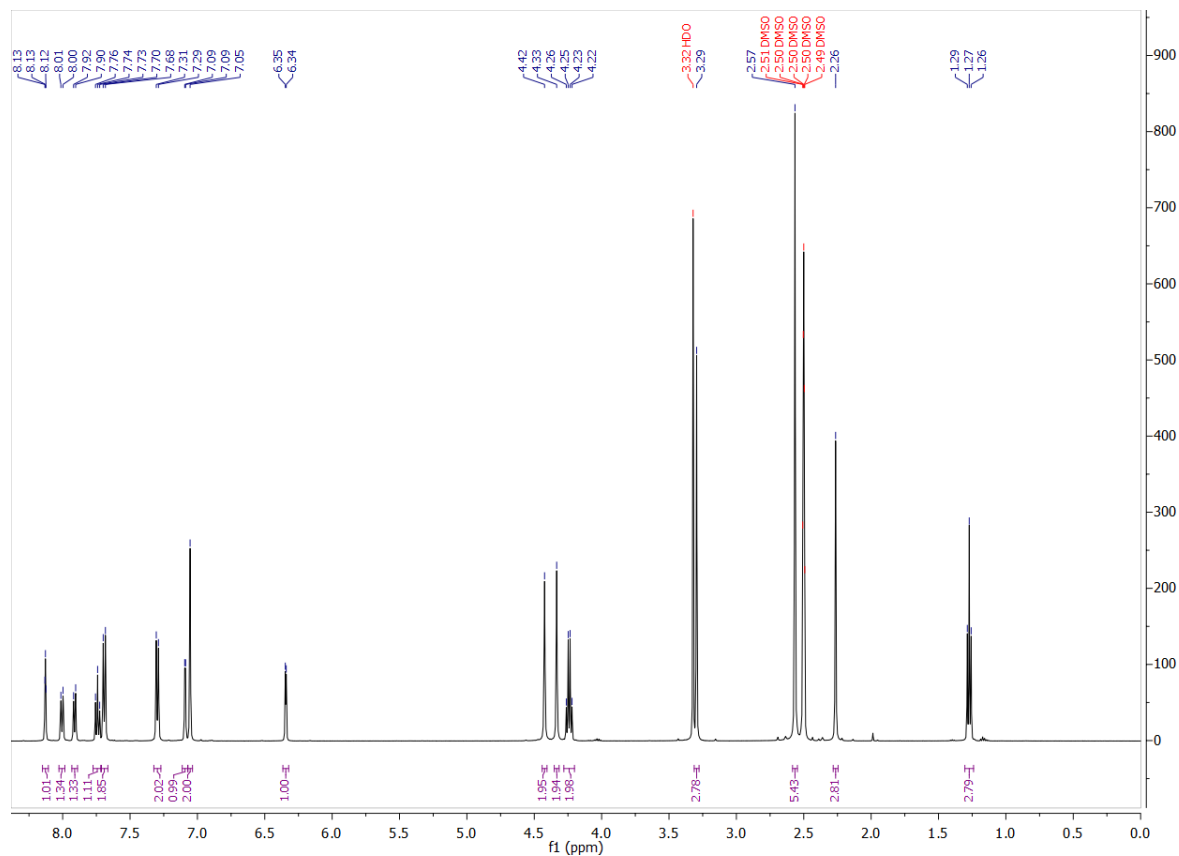


Biological activity

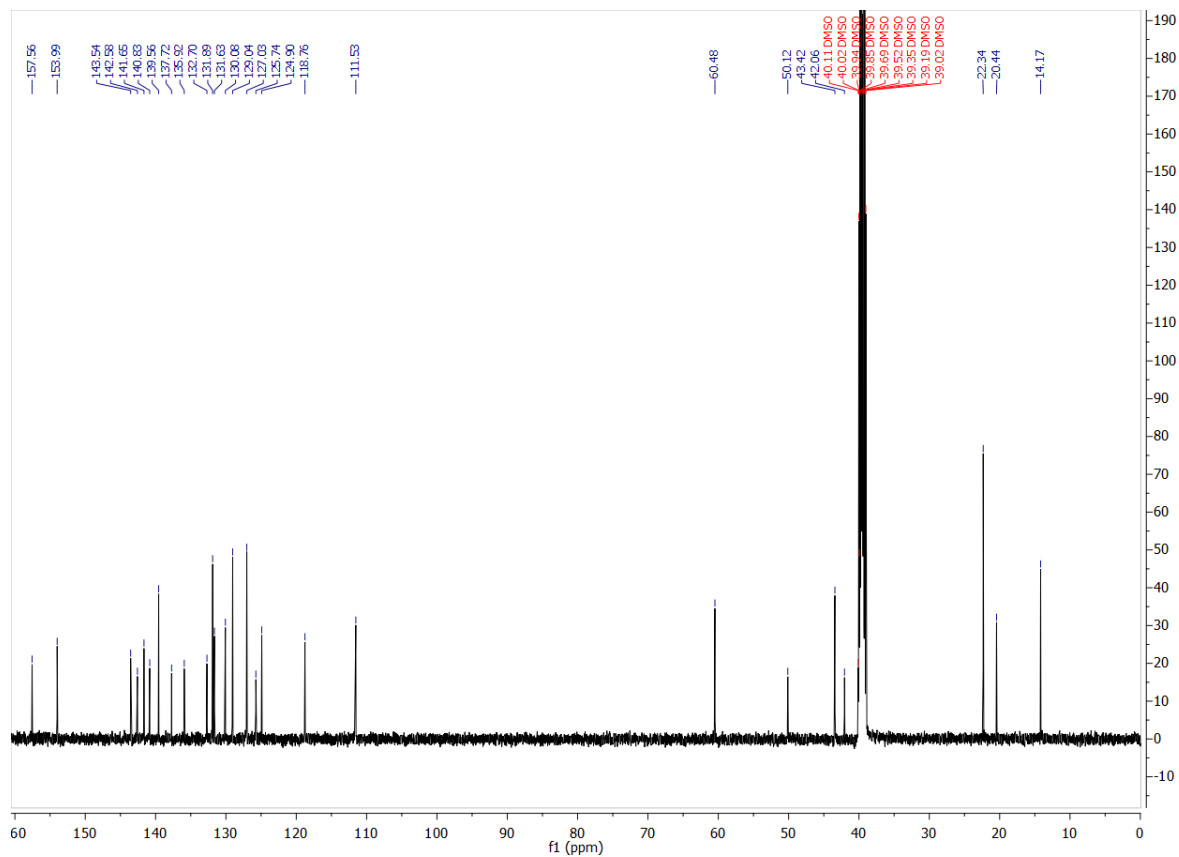
		Type	IC ₅₀ /EC ₅₀ [μM]	Reference
Main NR target:	NR1H3 (LXRα)	Antagonist	0.2	https://doi.org/10.1021/cb300541g
	NR1H2 (LXRβ)	Antagonist	0.04	
NR off-target:				

Identity

¹H NMR



¹³C NMR



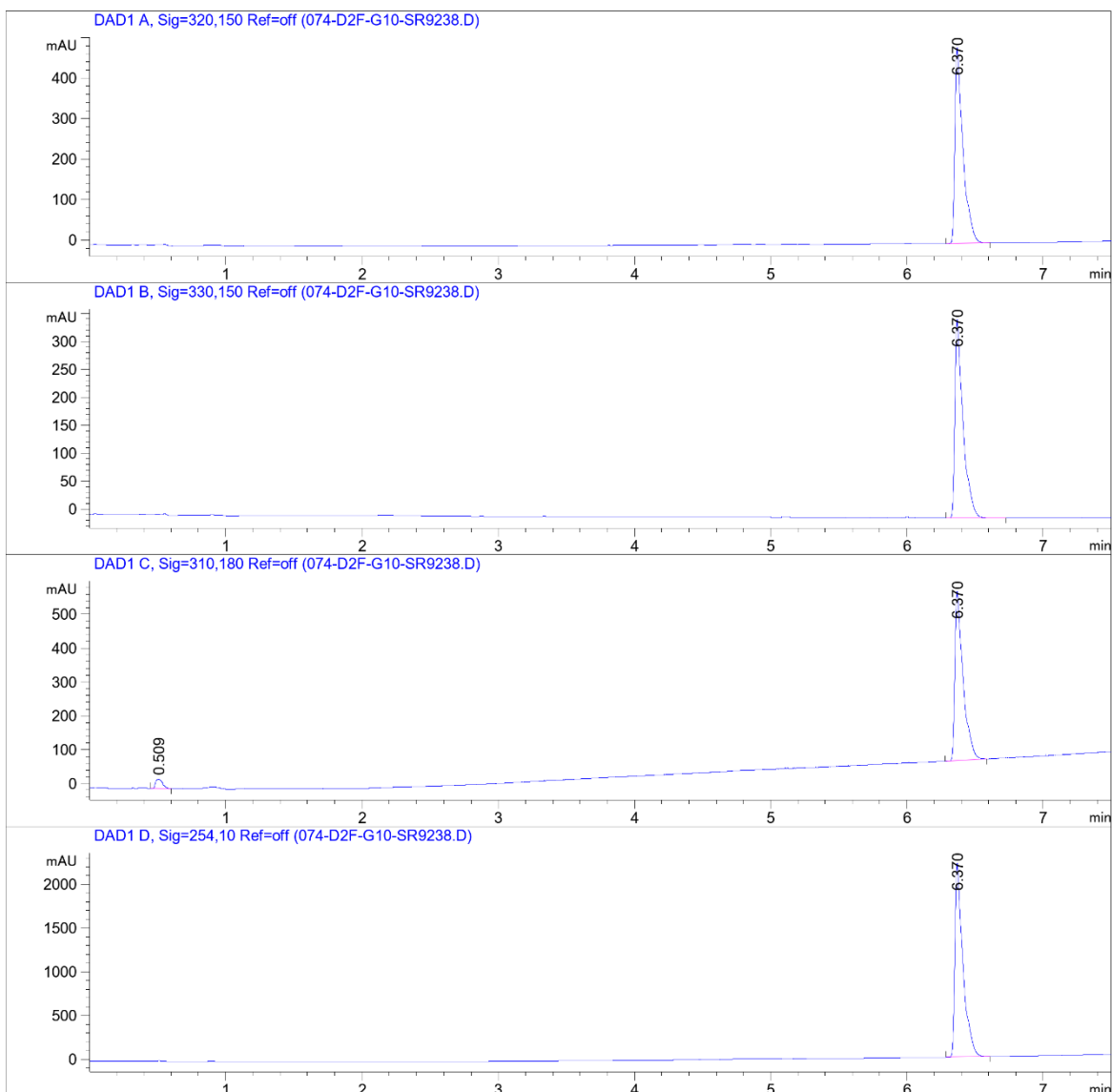
COMPOUND INFORMATION

Purity

Data File W:\analyti...PEN\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\074-D2F-G10-SR9238.D

Sample Name: SR9238

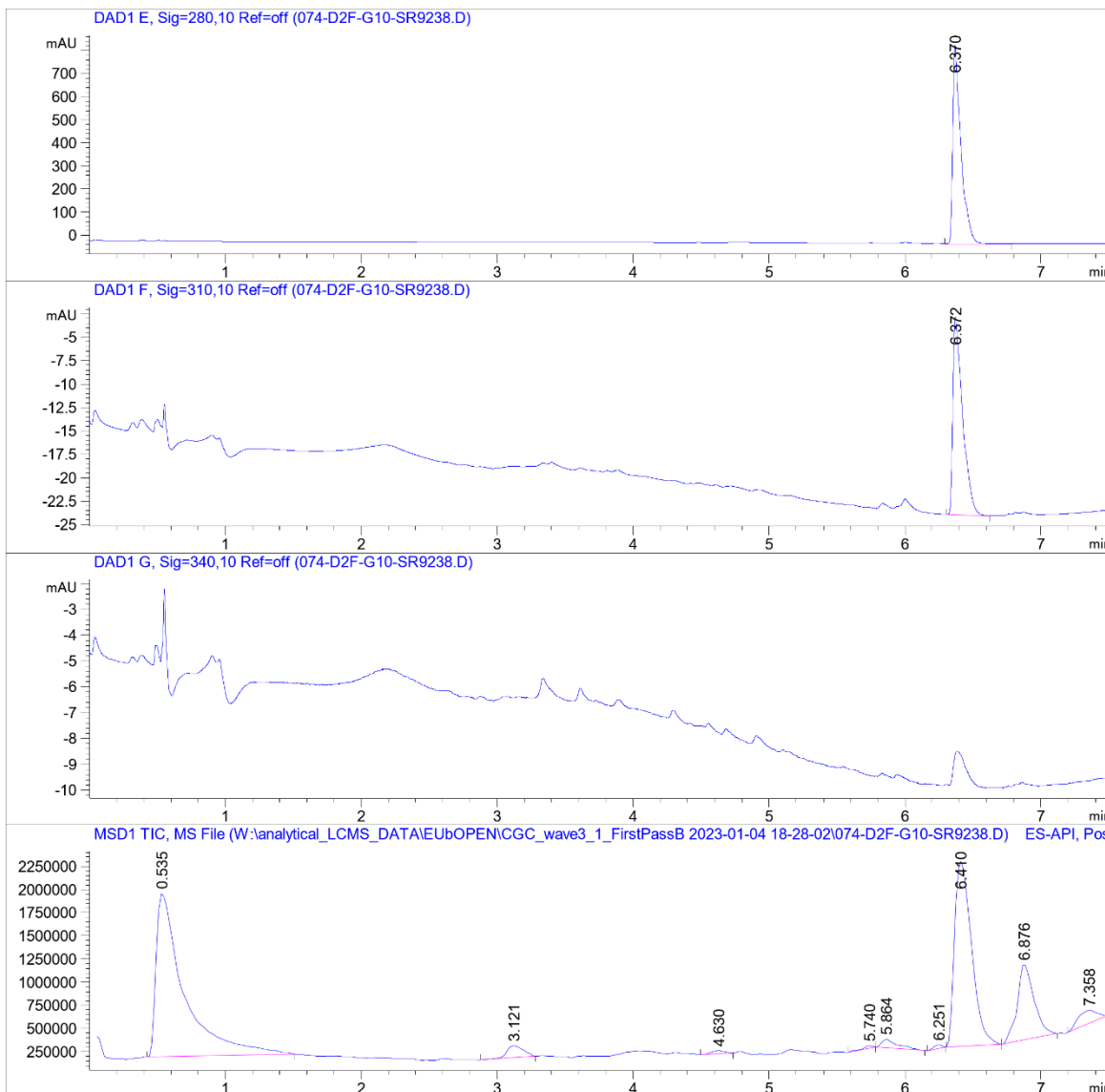
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=====
Acq. Operator   : SYSTEM                      Seq. Line :   74
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2F-G10
Injection Date  : 1/5/2023 7:58:03 AM        Inj       :    1
                                           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\074-D2F-G10-SR9238.D

Sample Name: SR9238



COMPOUND INFORMATION

Data File W:\analyti...PEN\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\074-D2F-G10-SR9238.D

Sample Name: SR9238

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	25013830	157.00 I
-	-	3.121	1090441	239.10 I 217.10 I
-	-	4.630	197414	510.40 I 170.90 I 158.20 I
-	-	5.740	127908	280.20 I
-	-	5.864	766346	318.20 I 296.20 I
-	-	6.251	149562	228.20 I 137.10 I
6.370	1972	6.410	17302958	618.20 I 596.20 I
-	-	6.876	6988443	282.20 I
-	-	7.358	1392870	400.30 I 282.20 I

