

GW0742

CAS Registry No.: 317318-84-6

Formal Name: 2-(4-(((2-(3-fluoro-4-(trifluoromethyl)phenyl)-4-methylthiazol-5-yl)methyl)thio)-2-methylphenoxy)acetic acid

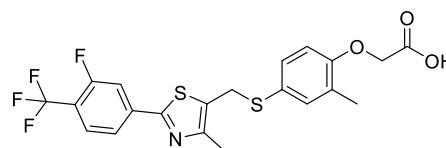
EUBOPEN ID: EUB0000569a

Molecular Formula: C₂₁H₁₇F₄NO₃S₂

Molecular Weight: 471.48 g/mol

Smiles: CC1=C(C=CC(=C1)SCC2=C(N=C(S2)C3=CC(=C(C=C3)C(F)(F)F)C)OCC(=O)O

Recommended concentration: 1 μM

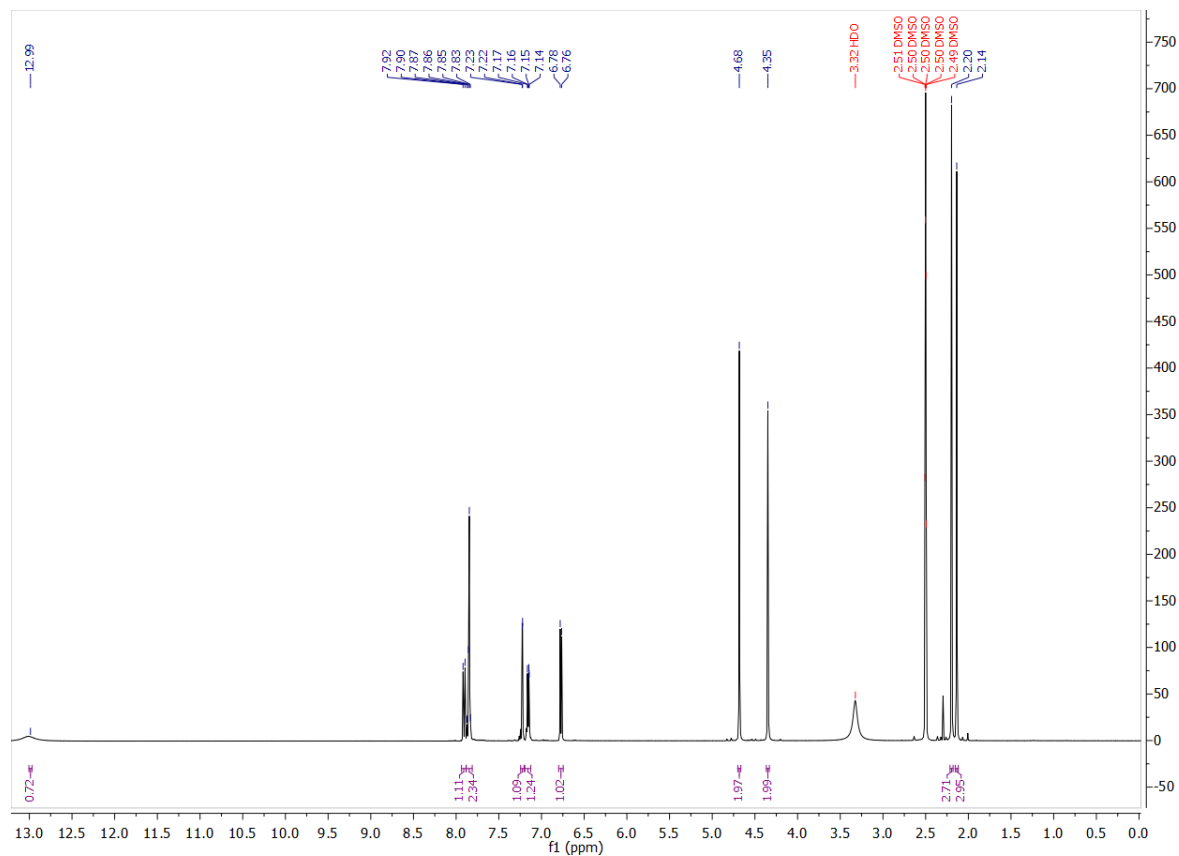


Biological activity

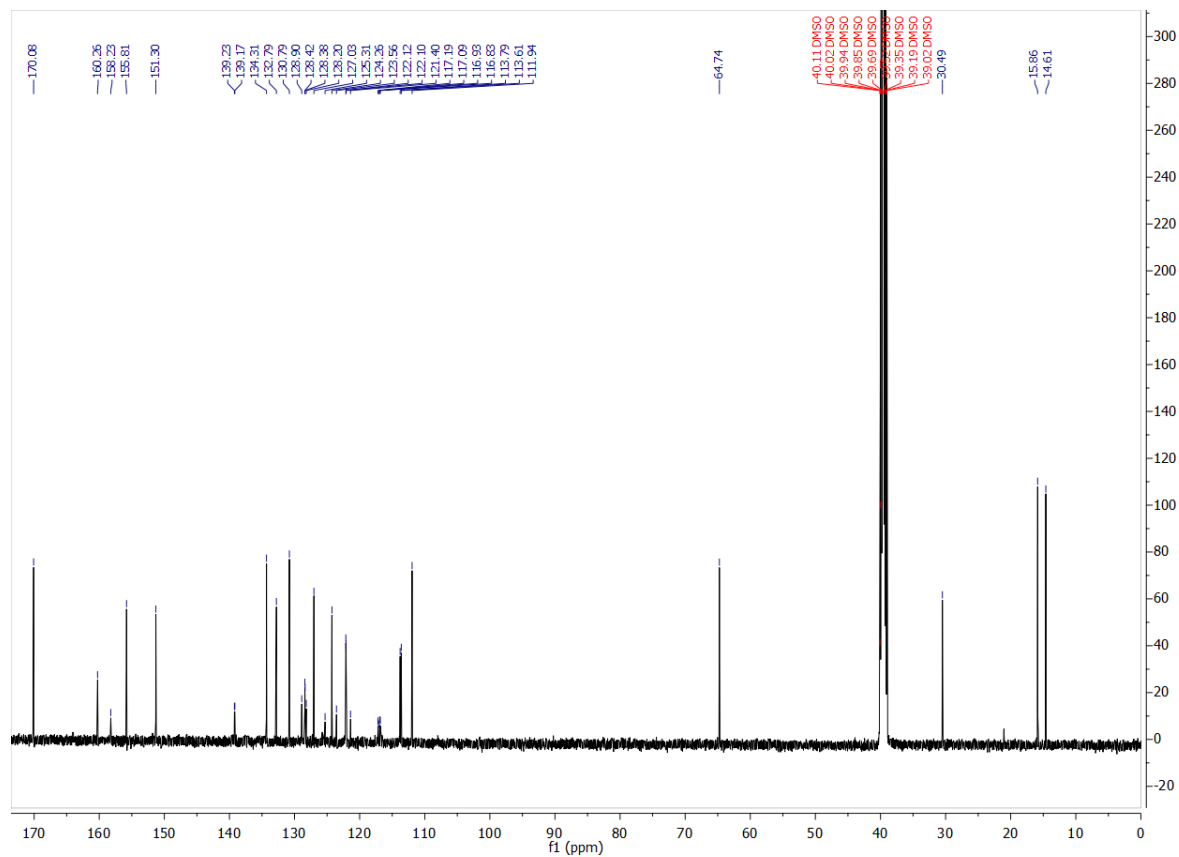
		Type	IC ₅₀ /EC ₅₀ [μM]	Reference
Main NR target:	NR1C2 (PPARδ)	Agonist	0.001	https://doi.org/10.1016/S0960-894X(03)00207-5
NR off-target:	NR1C1 (PPARα)	Agonist	1.1	https://doi.org/10.1016/S0960-894X(03)00207-5
	NR1C3 (PPARγ)	Agonist	2	

Identity

¹H NMR



¹³C NMR



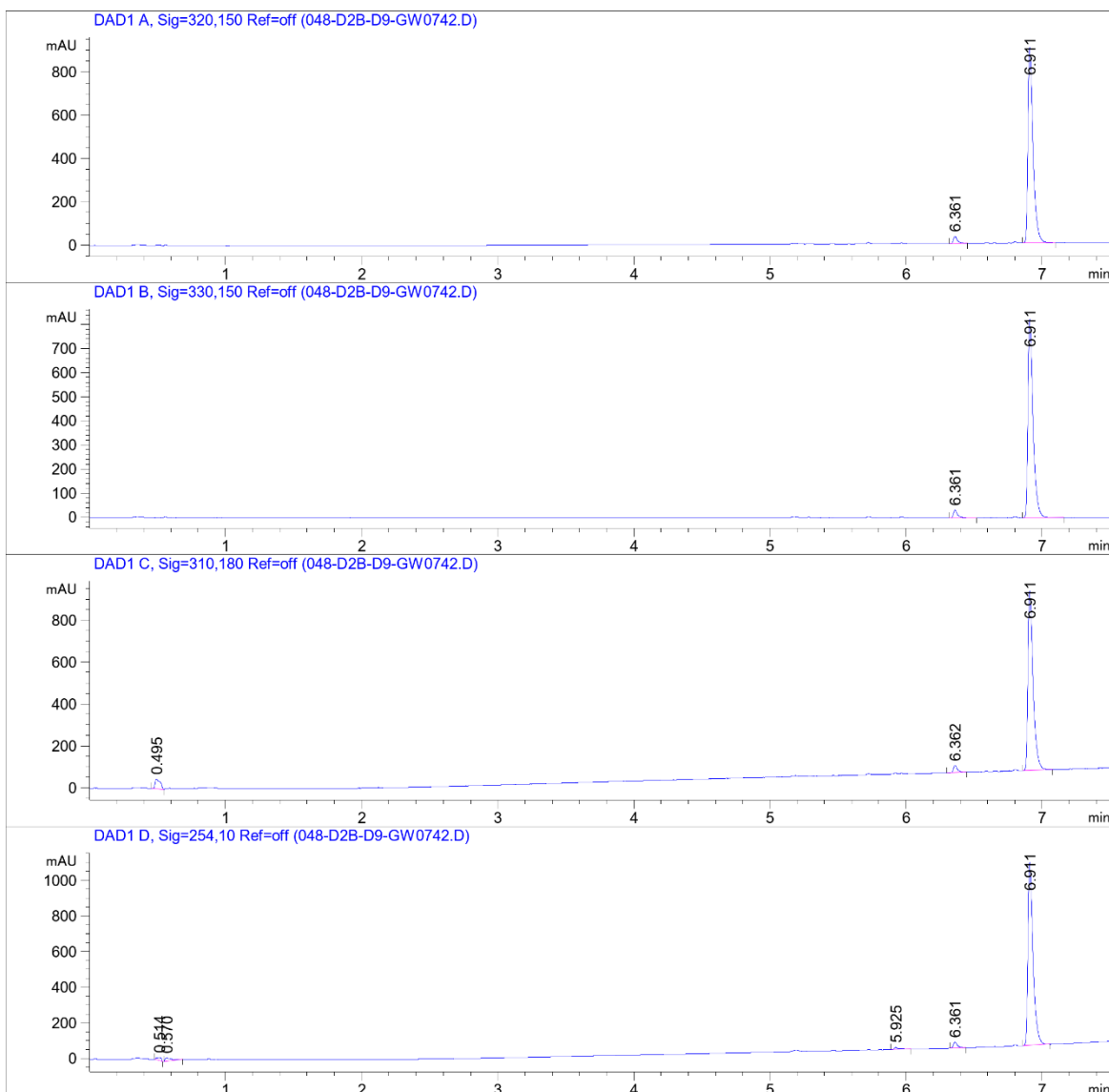
COMPOUND INFORMATION

Purity

Data File W:\analyti...bOPEN\CGC_ECH01-3_FirstPass 2021-03-20 13-21-54\048-D2B-D9-GW0742.D

Sample Name: GW0742

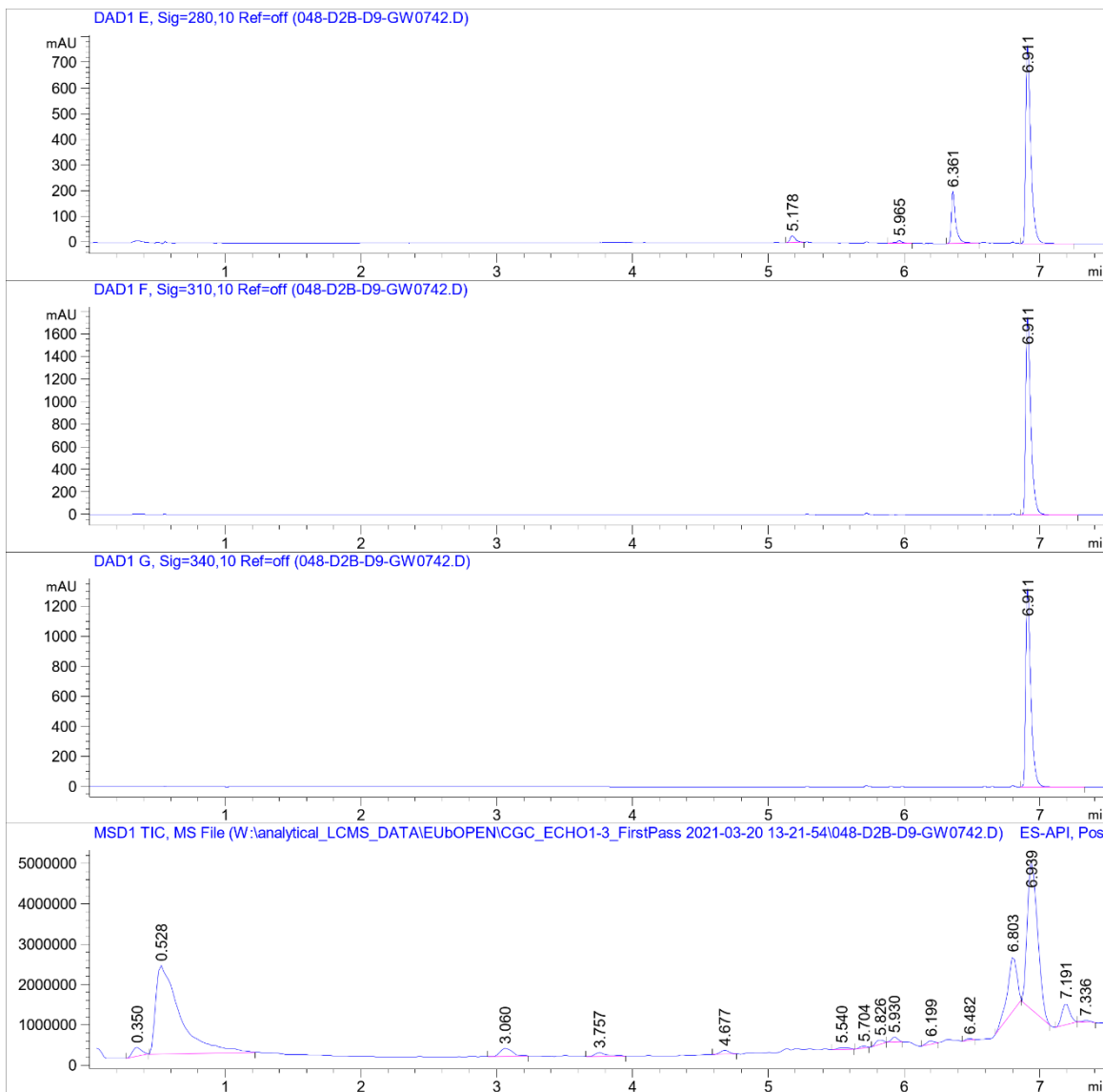
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=====
Acq. Operator   : SYSTEM                      Seq. Line :   48
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2B-D9
Injection Date  : 3/20/2021 10:06:29 PM      Inj       :    1
                                           Inj Volume: Inj prog
Sequence File   : W:\analytical_LCMS_DATA\EUBOPEN\CGC_ECH01-3_FirstPass 2021-03-20 13-21-54
                  \CGC_ECH01-3_FirstPass.S
Method          : W:\analytical_LCMS_DATA\EUBOPEN\CGC_ECH01-3_FirstPass 2021-03-20 13-21-54
                  \CGL_FIRSTPASS_GENERALMETHOD_VIAL3+4_20210319.M (Sequence Method)
Last changed    : 3/19/2021 5:35:24 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...bOPEN\CGC_ECHO1-3_FirstPass 2021-03-20 13-21-54\048-D2B-D9-GW0742.D

Sample Name: GW0742



COMPOUND INFORMATION

Data File W:\analyti...bOPEN\CGC_ECHO1-3_FirstPass 2021-03-20 13-21-54\048-D2B-D9-GW0742.D

Sample Name: GW0742

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
-	-	0.350	980700	182.90 I 158.00 I 130.00 I
-	-	0.528	27156862	157.00 I
-	-	3.060	1290951	217.00 I
-	-	3.757	597148	274.20 I
-	-	4.677	412555	326.40 I
-	-	5.540	251422	326.20 I 295.10 I 282.20 I 280.20 I 102.20 I
-	-	5.704	145791	280.20 I
-	-	5.826	403374	296.20 I
-	-	5.930	391858	296.20 I 294.10 I 280.20 I
-	-	6.199	286367	280.20 I 228.20 I
6.361	69	-	-	
-	-	6.482	158819	280.20 I
-	-	6.803	6534369	282.20 I
6.911	2347	6.939	19302544	472.10 I
-	-	7.191	2157972	284.30 I 282.20 I
-	-	7.336	192554	400.30 I 282.20 I

