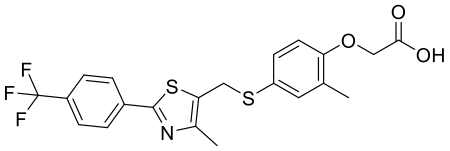
COMPOUND INFORMATION

GW501516

CAS Registry No.:	317318-70-0
Formal Name:	2-(2-methyl-4-(((4-methyl-2-(4-(trifluoromethyl)phenyl)thiazol-5-yl)methyl)thio)phenoxy)acetic acid
EUbOPEN ID:	EUB0001148a
Molecular Formula:	$C_{21}H_{18}F_3NO_3S_2$
Molecular Weight:	453.49 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



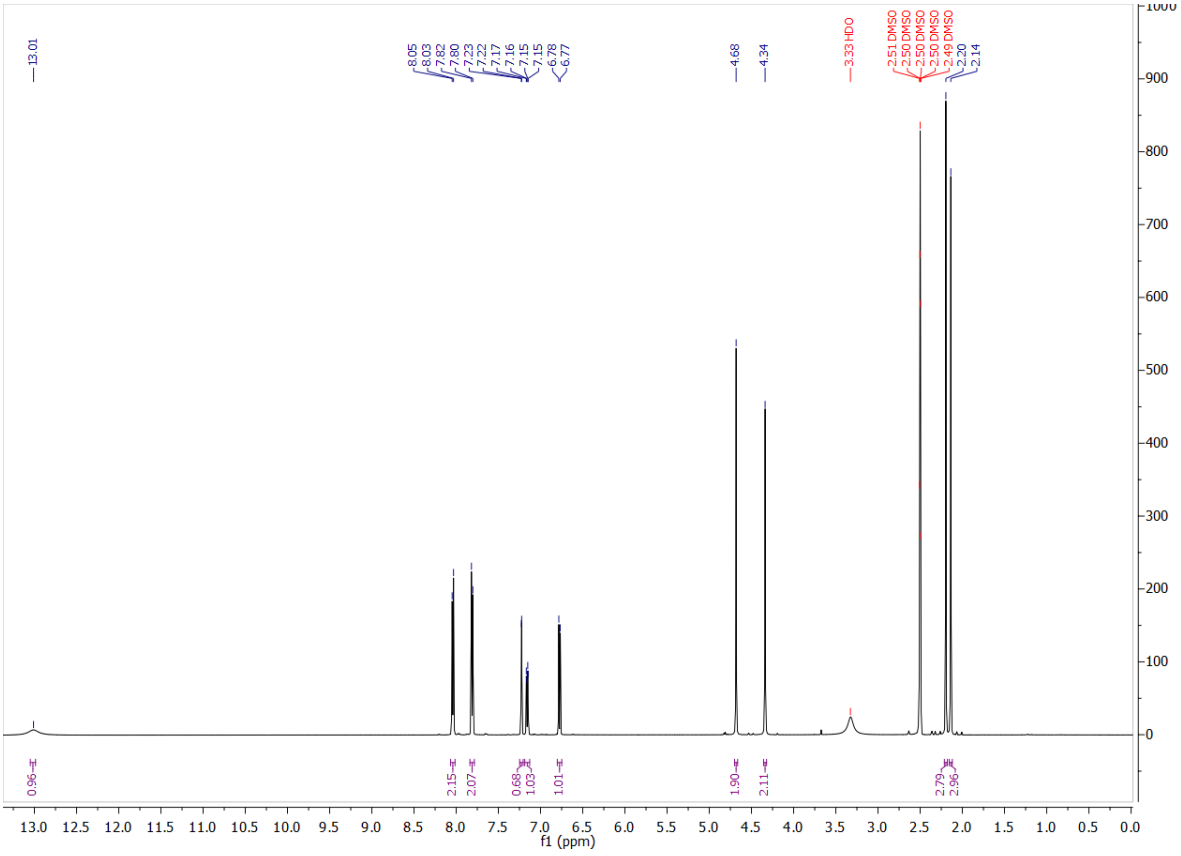
Biological activity

		Type	IC_{50}/EC_{50} [µM]	Reference
Main NR target:	NR1C2 (PPARδ)	Agonist	0.001	https://doi.org/10.1073/pnas.091021198
NR off-target:				

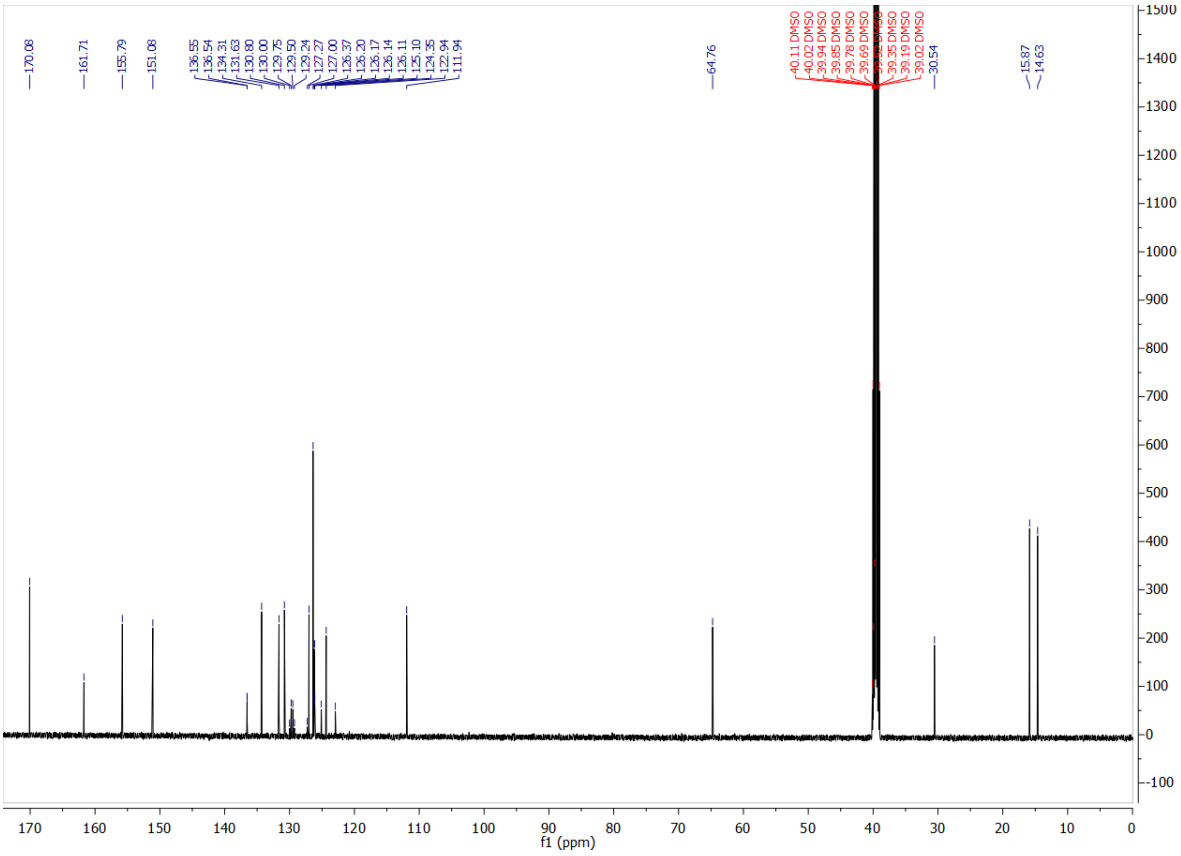
COMPOUND INFORMATION

Identity

^{1}H NMR



^{13}C NMR



COMPOUND INFORMATION

Purity

Data File W:\analyti...N\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\069-D2F-F6-GW 501516.D
Sample Name: GW 501516

```
======================================================================
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Sample Operator : SYSTEM
Acq. Instrument : LCMS test                      Location :   D2F-F6
Injection Date  : 1/5/2023 7:02:46 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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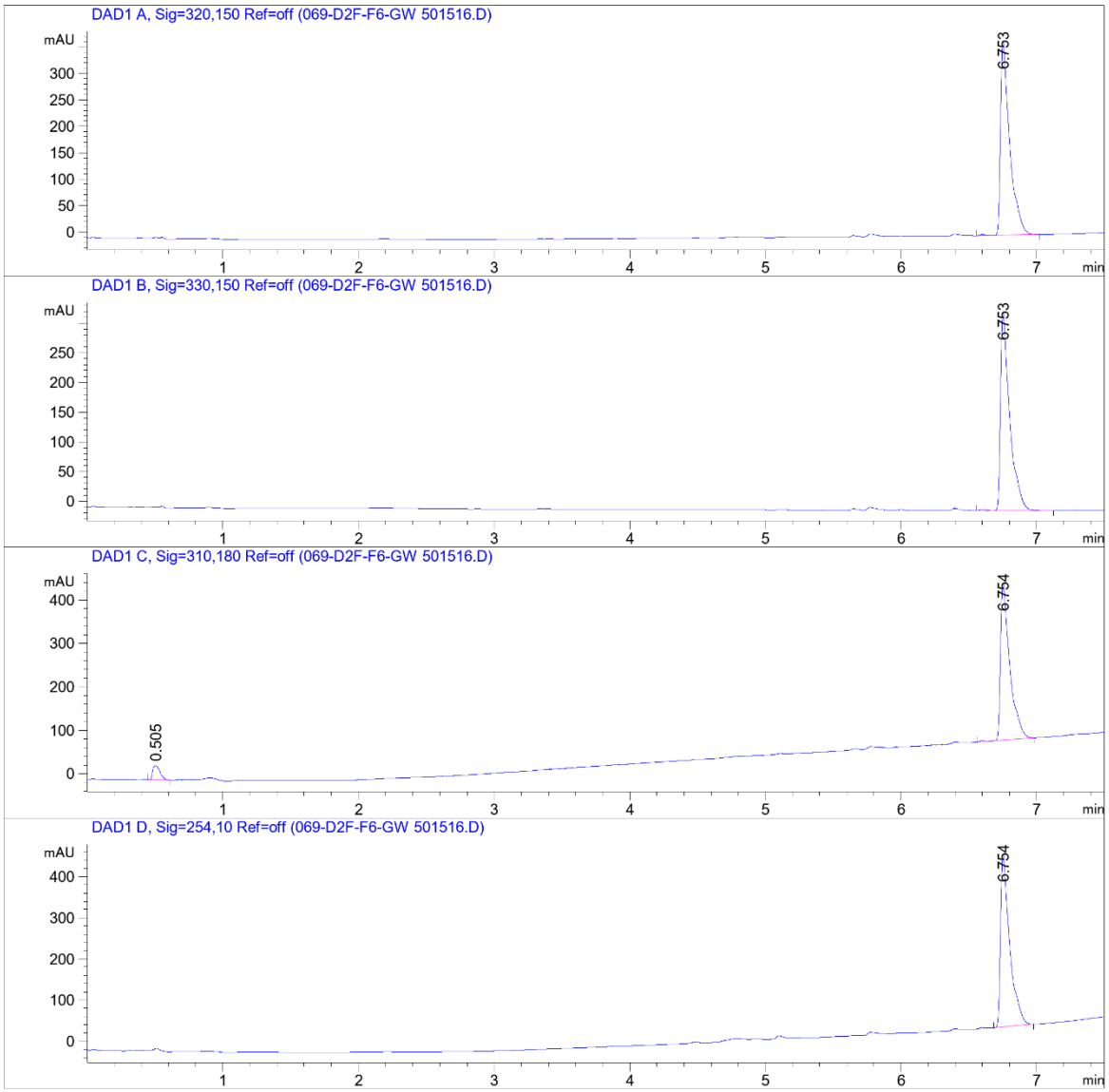
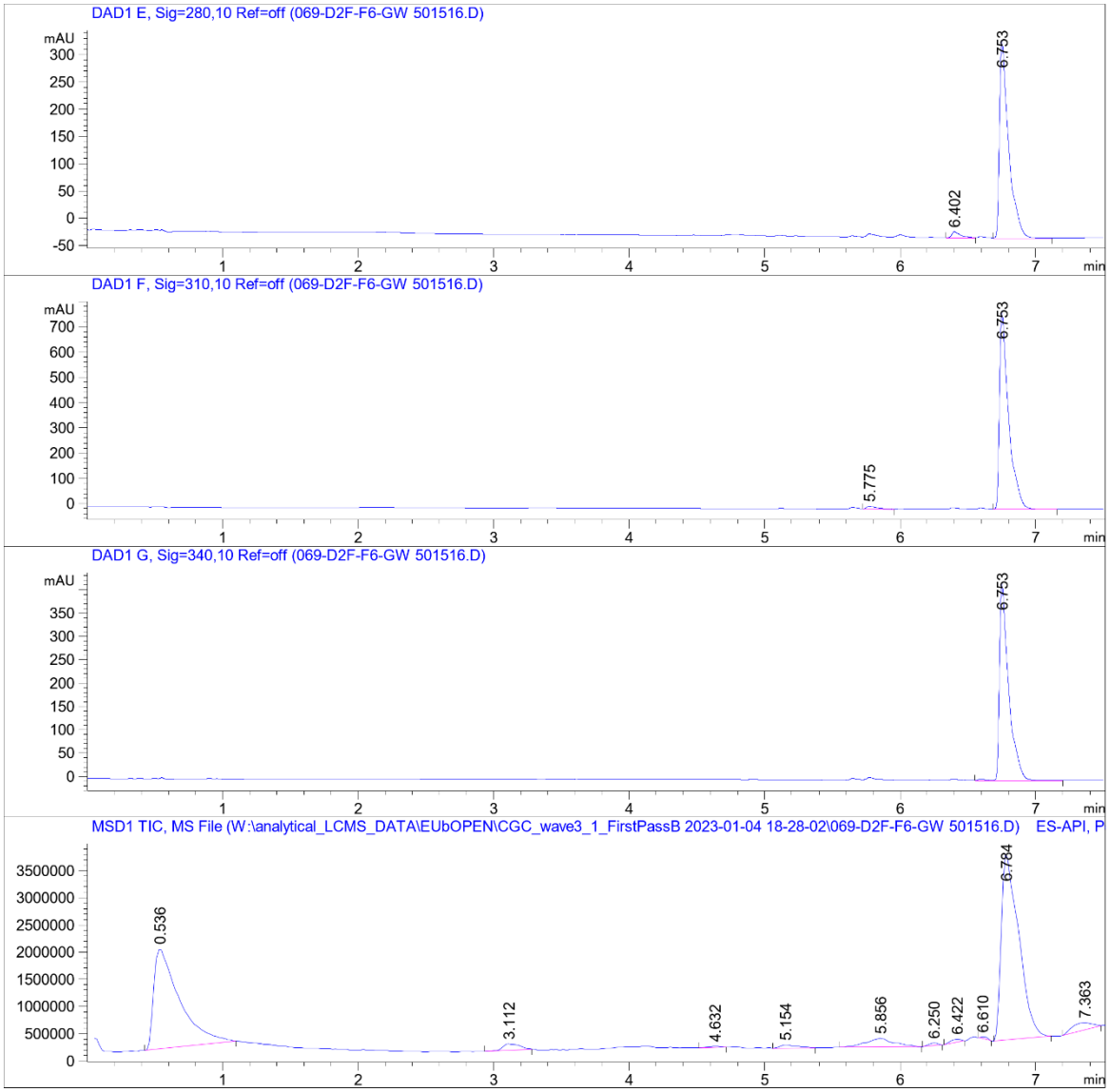


COMPOUND INFORMATION

Data File W:\analyti...N\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\069-D2F-F6-GW 501516.D
Sample Name: GW 501516



COMPOUND INFORMATION

Data File W:\analyti...N\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\069-D2F-F6-GW 501516.D
Sample Name: GW 501516

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
-	-	0.536	24070416	157.00 I
-	-	3.112	1019263	239.00 I
				217.10 I
-	-	4.632	164508	510.40 I
				170.80 I
				158.10 I
-	-	5.154	578058	510.30 I
				274.00 I
				170.90 I
				137.10 I
-	-	5.856	2261523	318.20 I
				296.20 I
-	-	6.250	216604	228.20 I
				137.10 I
-	-	6.422	326089	436.10 I
				350.20 I
				282.30 I
				254.20 I
				137.20 I
-	-	6.610	133779	507.30 I
				468.00 I
				280.20 I
6.753	1709	6.784	30612550	454.10 I
-	-	7.363	1397508	400.30 I
				282.30 I