

GW3965 (hydrochloride)

CAS Registry No.: 405911-17-3

Formal Name: 2-(3-(3-((2-chloro-3-(trifluoromethyl)benzyl)(2,2-diphenylethyl)amino)propoxy)phenyl)acetic acid hydrochloride

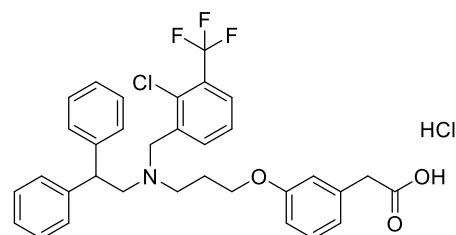
EUBOPEN ID: EUB0000572aCl

Molecular Formula: C₃₃H₃₂Cl₂F₃NO₃

Molecular Weight: 618.52 g/mol

Smiles: O=C(O)CC1=CC(OCCCN(CC2=C(Cl)C(C(F)(F)F)=CC=C2)CC(C3=CC=CC=C3)C4=CC=CC=C4)=CC=C1.Cl

Recommended concentration: 3 µM

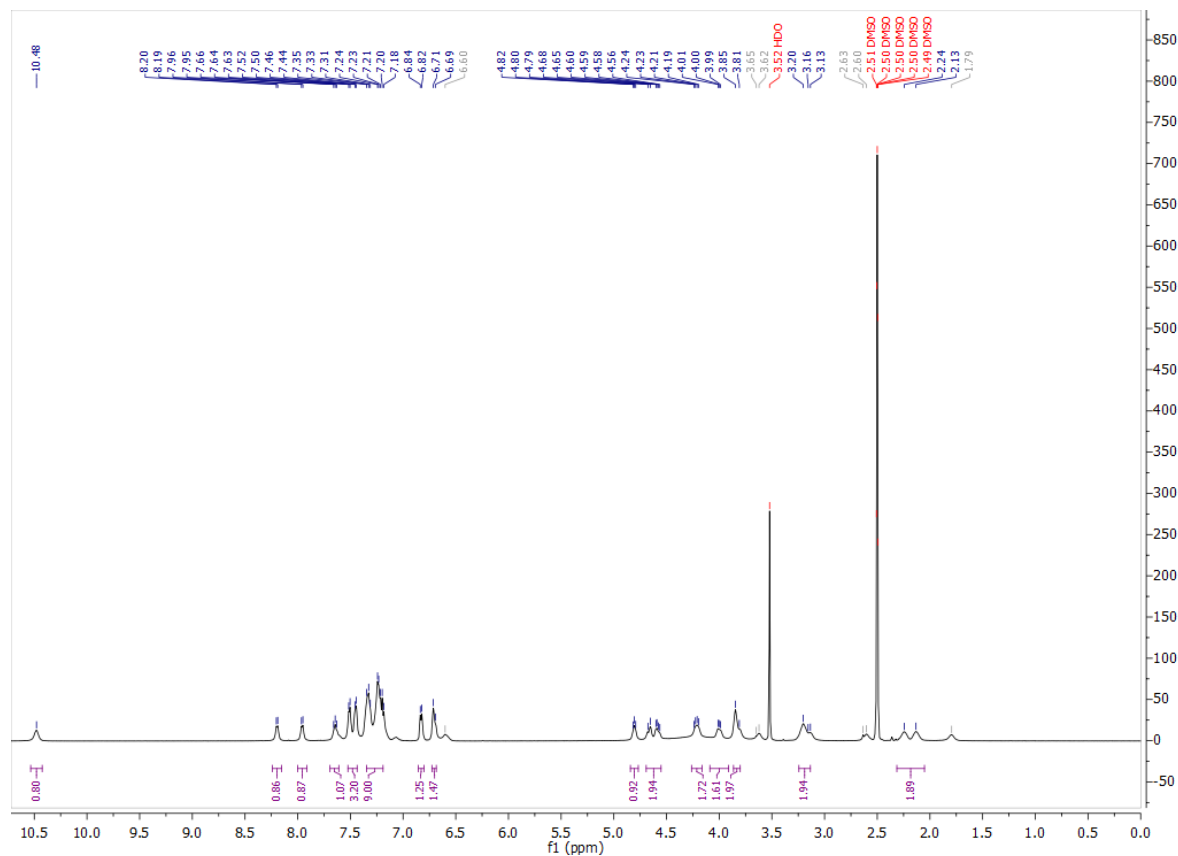


Biological activity

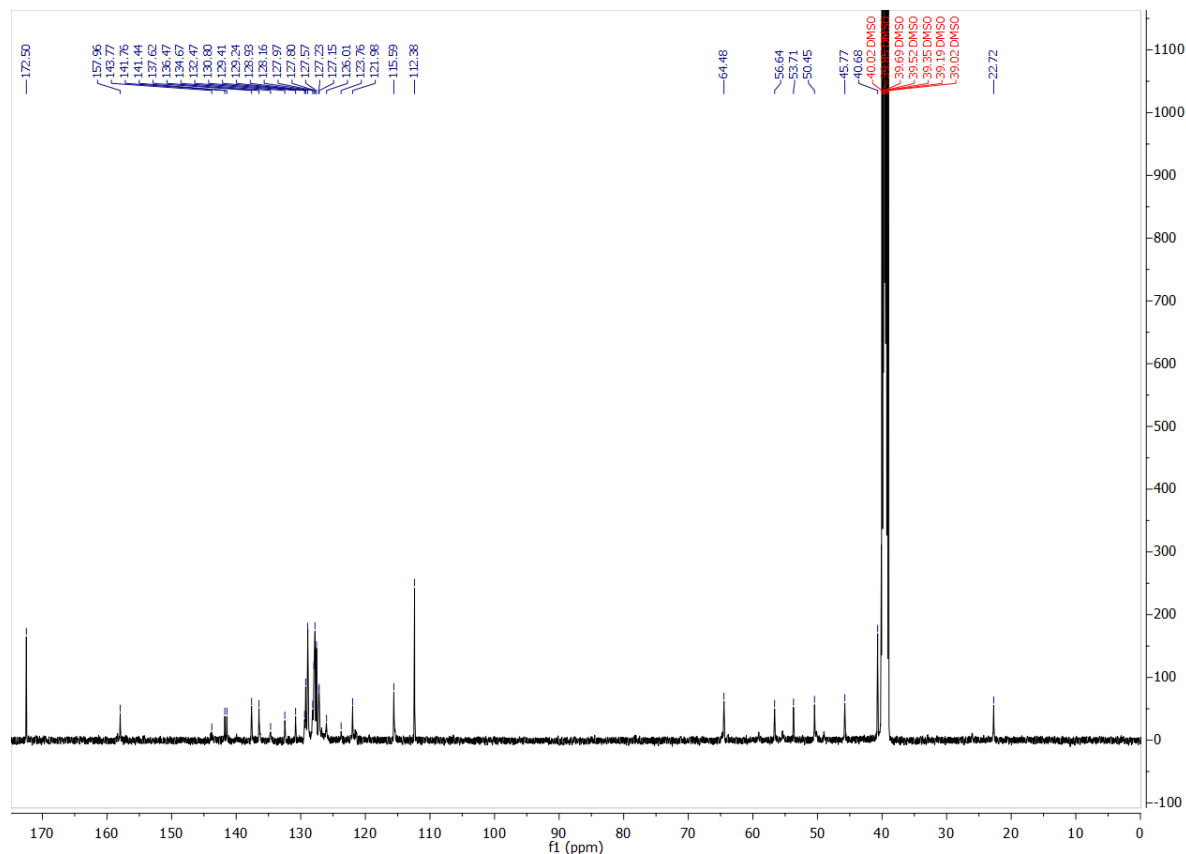
		Type	IC ₅₀ /EC ₅₀ [µM]	Reference
Main NR target:	NR1H3 (LXRα)	Agonist	0.19	https://doi.org/10.1021/jm0255116
	NR1H2 (LXRβ)	Agonist	2.1	inhouse
NR off-target:				

Identity

¹H NMR



¹³C NMR



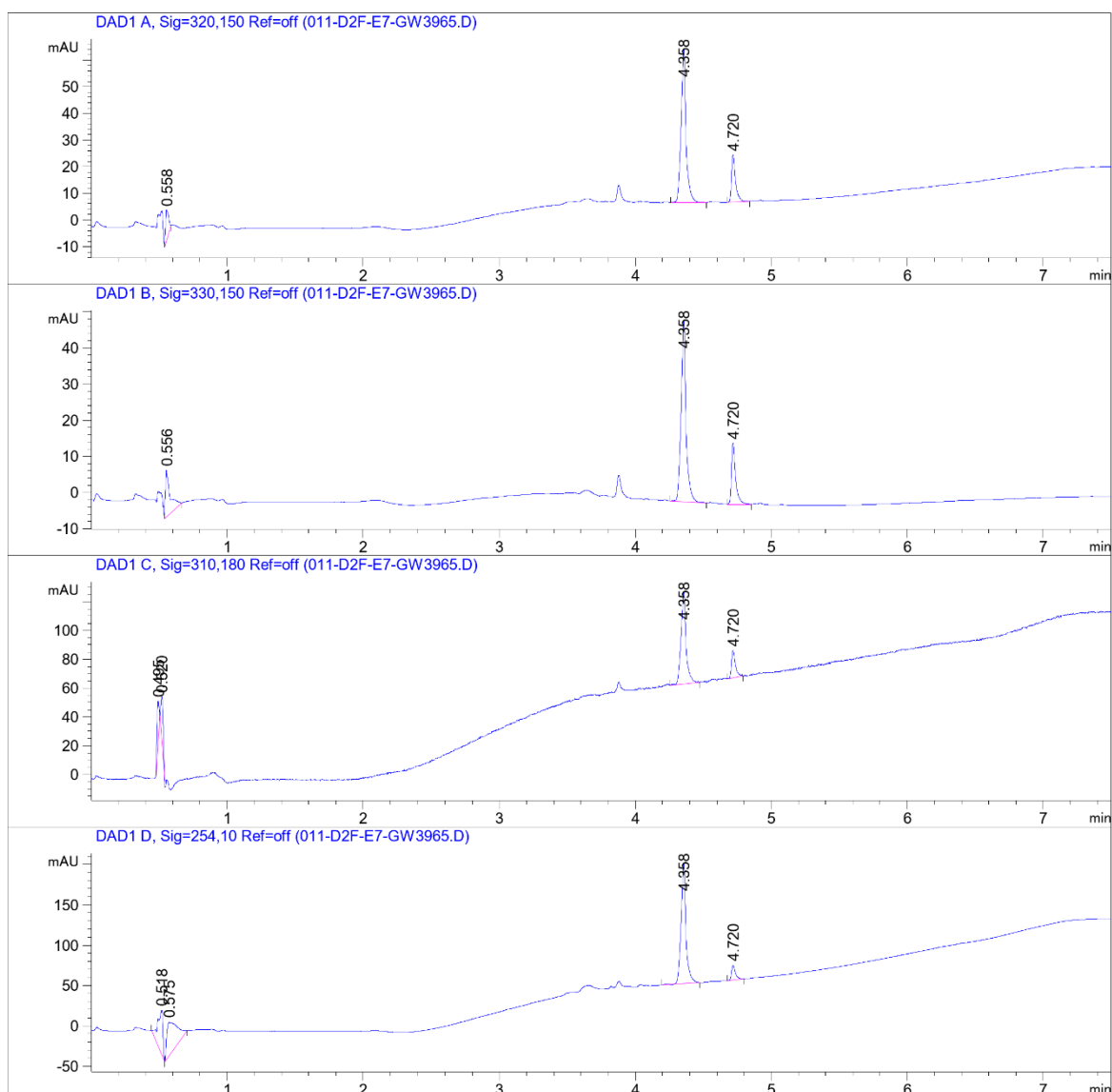
COMPOUND INFORMATION

Purity

Data File W:\analyti...OPEN\CGC_ECH01-3_SecondPass 2021-03-25 18-09-21\011-D2F-E7-GW3965.D

Sample Name: GW3965

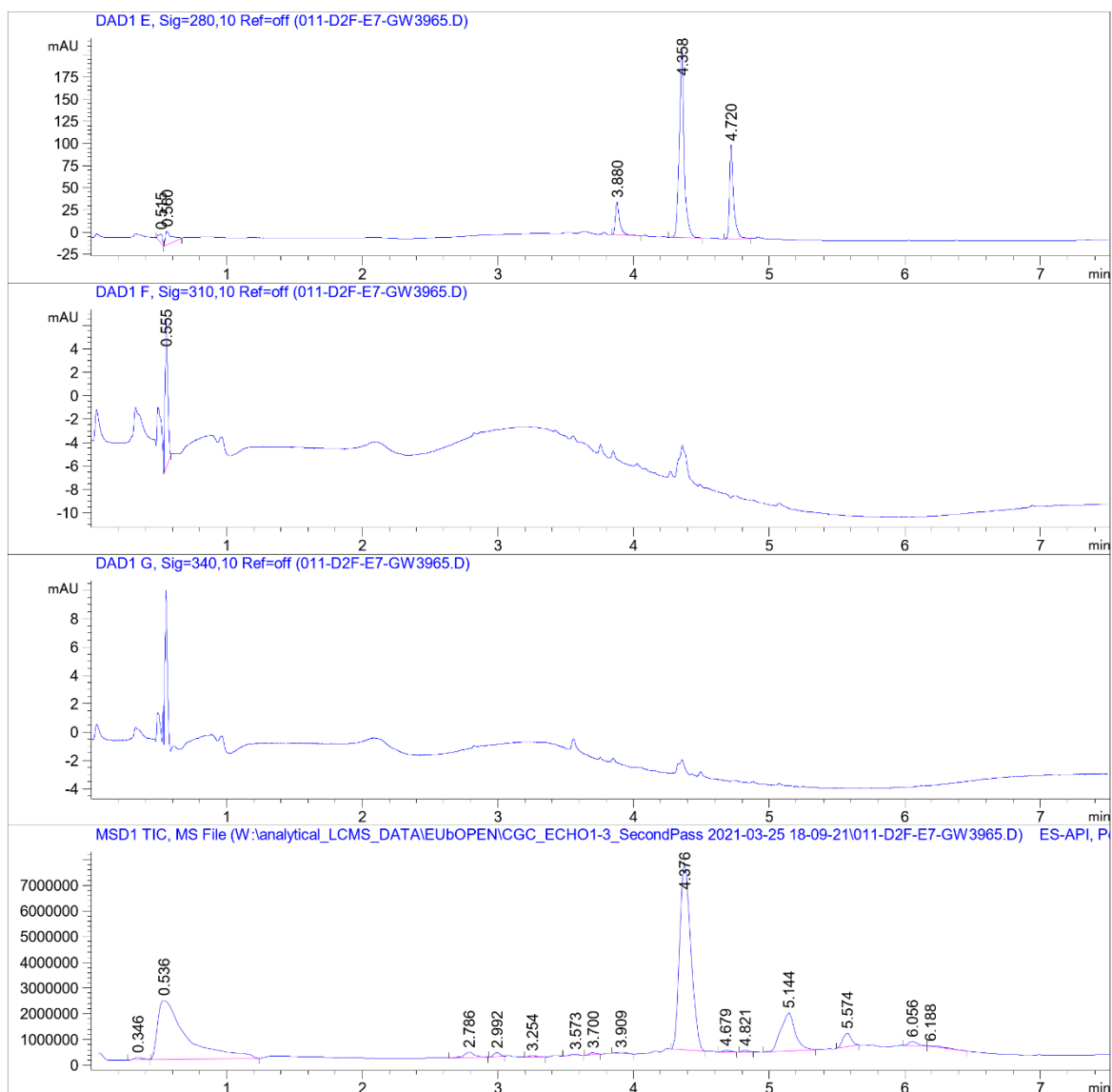
```
=====
Acq. Operator   : SYSTEM                      Seq. Line :   11
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2F-E7
Injection Date  : 3/25/2021 8:02:31 PM        Inj       :    1
                                           Inj Volume: Inj prog
Sequence File   : W:\analytical_LCMS_DATA\EUBOPEN\CGC_ECH01-3_SecondPass 2021-03-25 18-09-21
                  \CGC_ECH01-3_SecondPass.S
Method          : W:\analytical_LCMS_DATA\EUBOPEN\CGC_ECH01-3_SecondPass 2021-03-25 18-09-21
                  \CGL_SECONDPASS_NONPOLCOMP_VIAL2+4_20210323.M (Sequence Method)
Last changed    : 3/25/2021 4:32:02 PM by SYSTEM
Method Info     : CGL wellplate, 0.5 uL of 10 mM DMSO. Dilution with MeCN only (9+9 uL)
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COMPOUND INFORMATION

Data File W:\analyti...OPEN\CGC_ECH01-3_SecondPass 2021-03-25 18-09-21\011-D2F-E7-GW3965.D

Sample Name: GW3965



COMPOUND INFORMATION

Data File W:\analyti...OPEN\CGC_ECHO1-3_SecondPass 2021-03-25 18-09-21\011-D2F-E7-GW3965.D

Sample Name: GW3965

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

Spectra from peak tops.

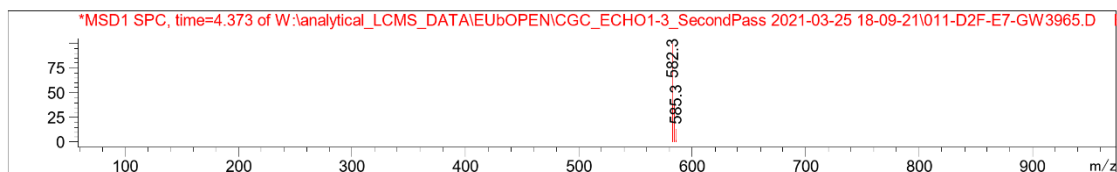
Noise Cutoff: 1000 counts.

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
-	-	0.346	376675	200.00 I 183.00 I 159.00 I
0.558	17	0.536	33732896	157.10 I
-	-	2.786	1132223	217.10 I
-	-	2.992	468838	274.30 I
-	-	3.254	289581	448.20 I
-	-	3.573	271154	224.10 I 111.10 I
-	-	3.700	304169	312.20 I 214.10 I
-	-	3.909	247316	512.50 I
4.358	145	4.376	42142564	582.30 I
4.720	36	4.679	302282	254.30 I
-	-	4.821	248968	280.20 I
-	-	5.144	10709928	282.30 I
-	-	5.574	2316434	381.30 I 359.30 I 341.30 I 284.30 I 282.30 I
-	-	6.056	715062	338.30 I 282.30 I
-	-	6.188	388252	282.30 I



COMPOUND INFORMATION

Biological activity

