

## GW7647

**CAS Registry No.:** 265129-71-3

**Formal Name:** 2-((4-(2-(3-cyclohexyl-1-(4-cyclohexylbutyl)ureido)ethyl)phenyl)thio)-2-methylpropanoic acid

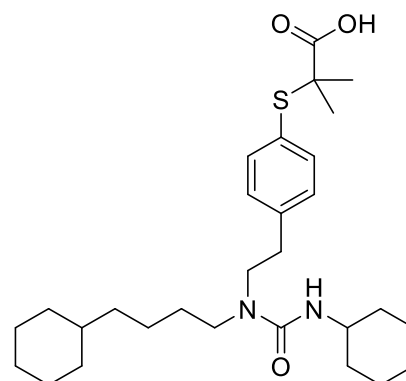
**EUbOPEN ID:** EUB0000185b

**Molecular Formula:** C<sub>29</sub>H<sub>46</sub>N<sub>2</sub>O<sub>3</sub>S

**Molecular Weight:** 502.76 g/mol

**Smiles:**  
CC(C)(C(=O)O)SC1=CC=C(C=C1)CCN(CCCCC2CCCCC2)C(=O)NC3CCCCC3

**Recommended concentration:** 1 μM

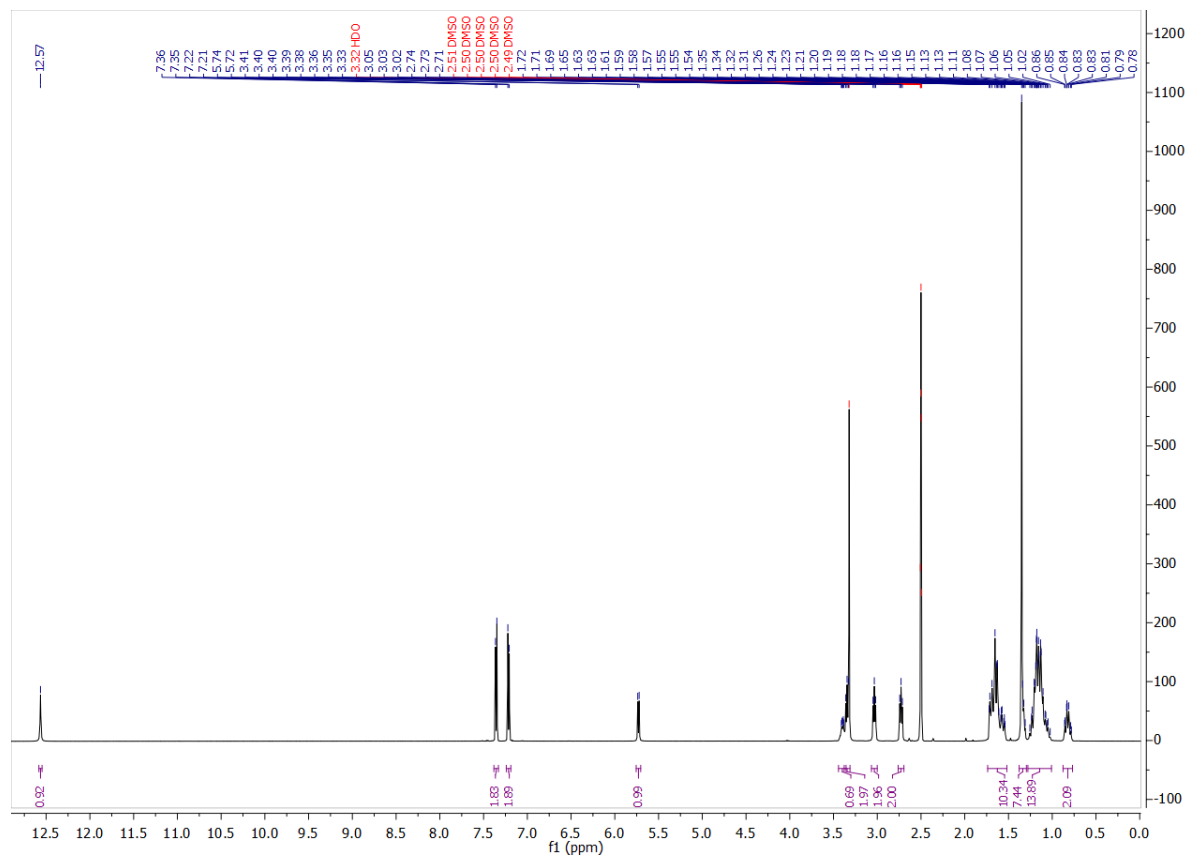


### Biological activity

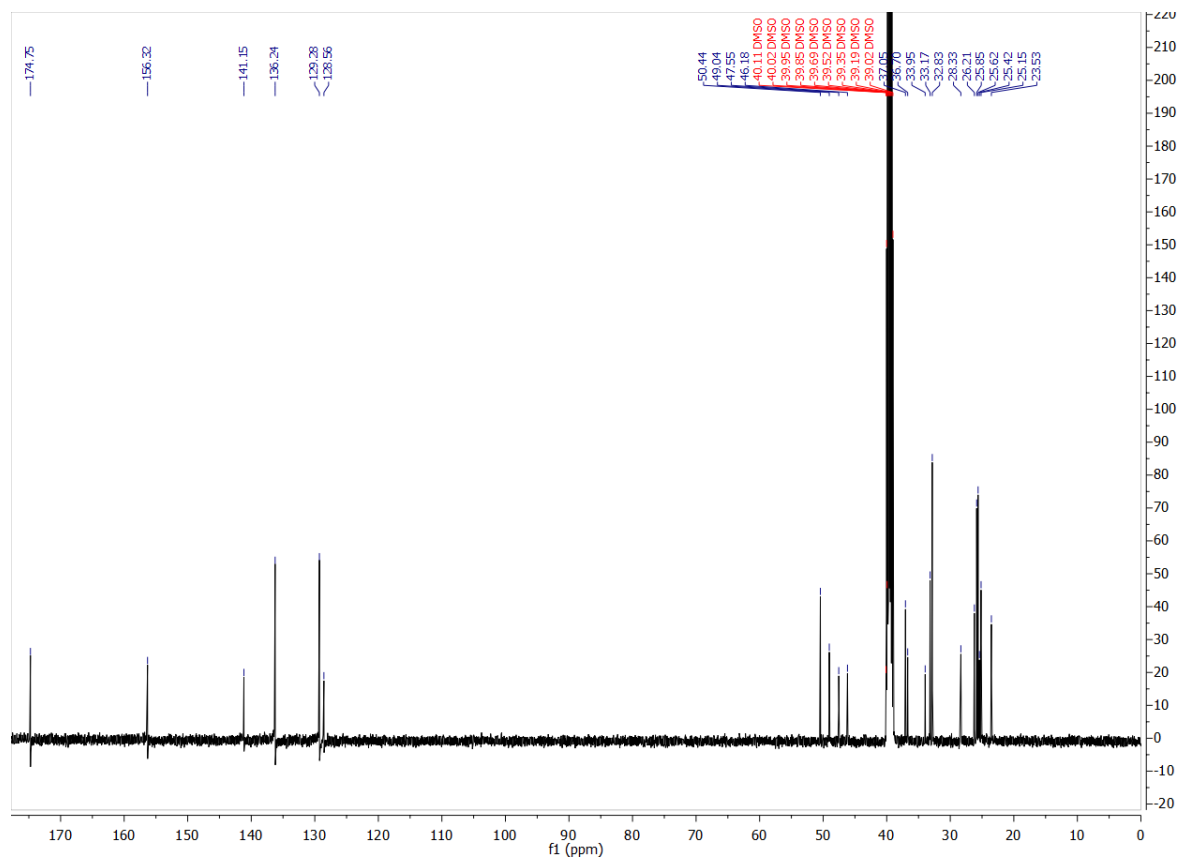
		Type	IC <sub>50</sub> /EC <sub>50</sub> [μM]	Reference
Main NR target:	NR1C1 (PPARα)	Agonist	0.006	<a href="https://doi.org/10.1016/S0960-894X(01)00188-3">https://doi.org/10.1016/S0960-894X(01)00188-3</a>
	NR1C3 (PPARγ)	Agonist	1	
NR off-target:	NR1C2 (PPARδ)	Agonist	6	<a href="https://doi.org/10.1016/S0960-894X(01)00188-3">https://doi.org/10.1016/S0960-894X(01)00188-3</a>

## Identity

### <sup>1</sup>H NMR



### <sup>13</sup>C NMR



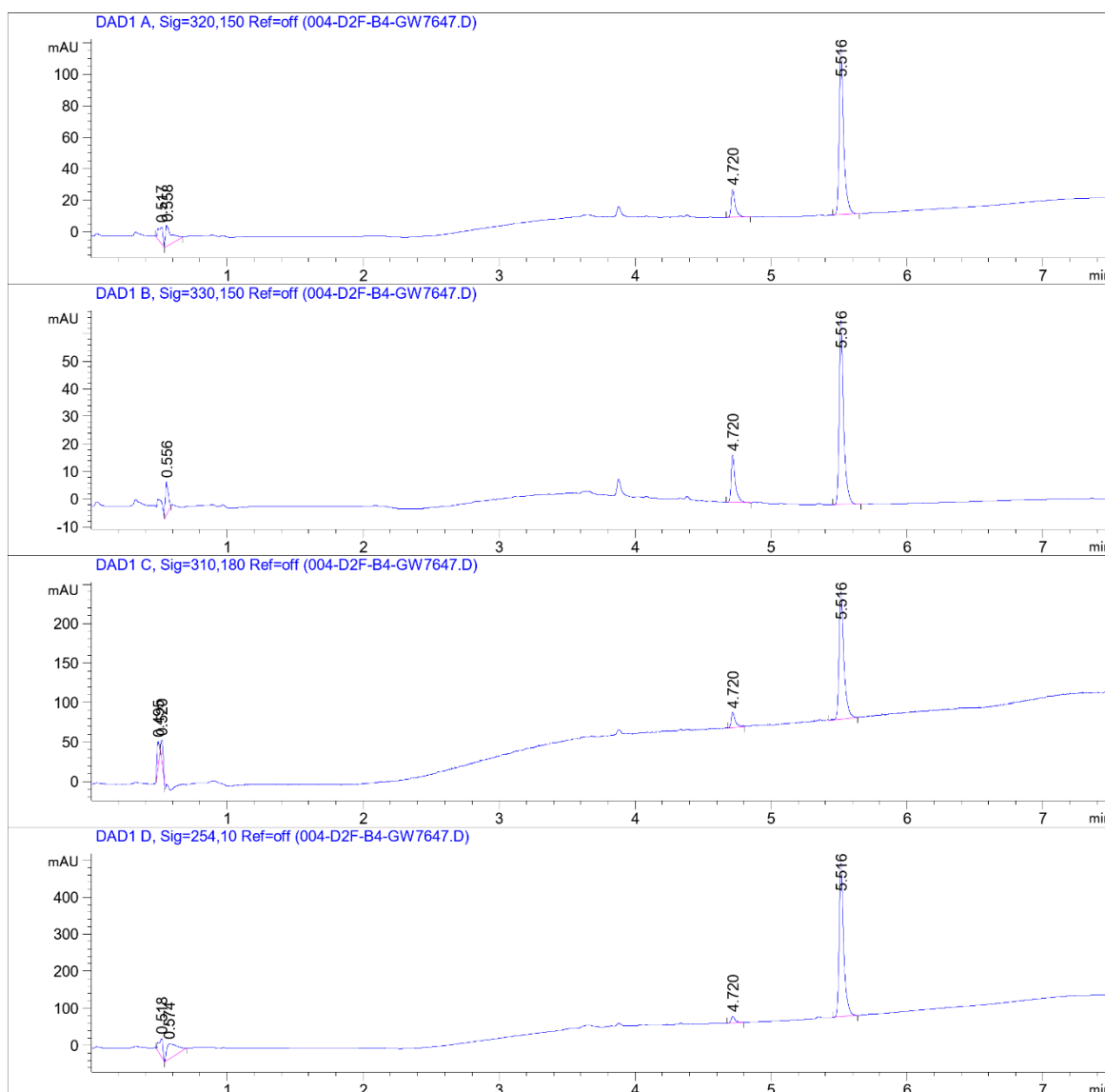
# COMPOUND INFORMATION

## Purity

Data File W:\analyti...OPEN\CGC\_ECH01-3\_SecondPass 2021-03-25 18-09-21\004-D2F-B4-GW7647.D

Sample Name: GW7647

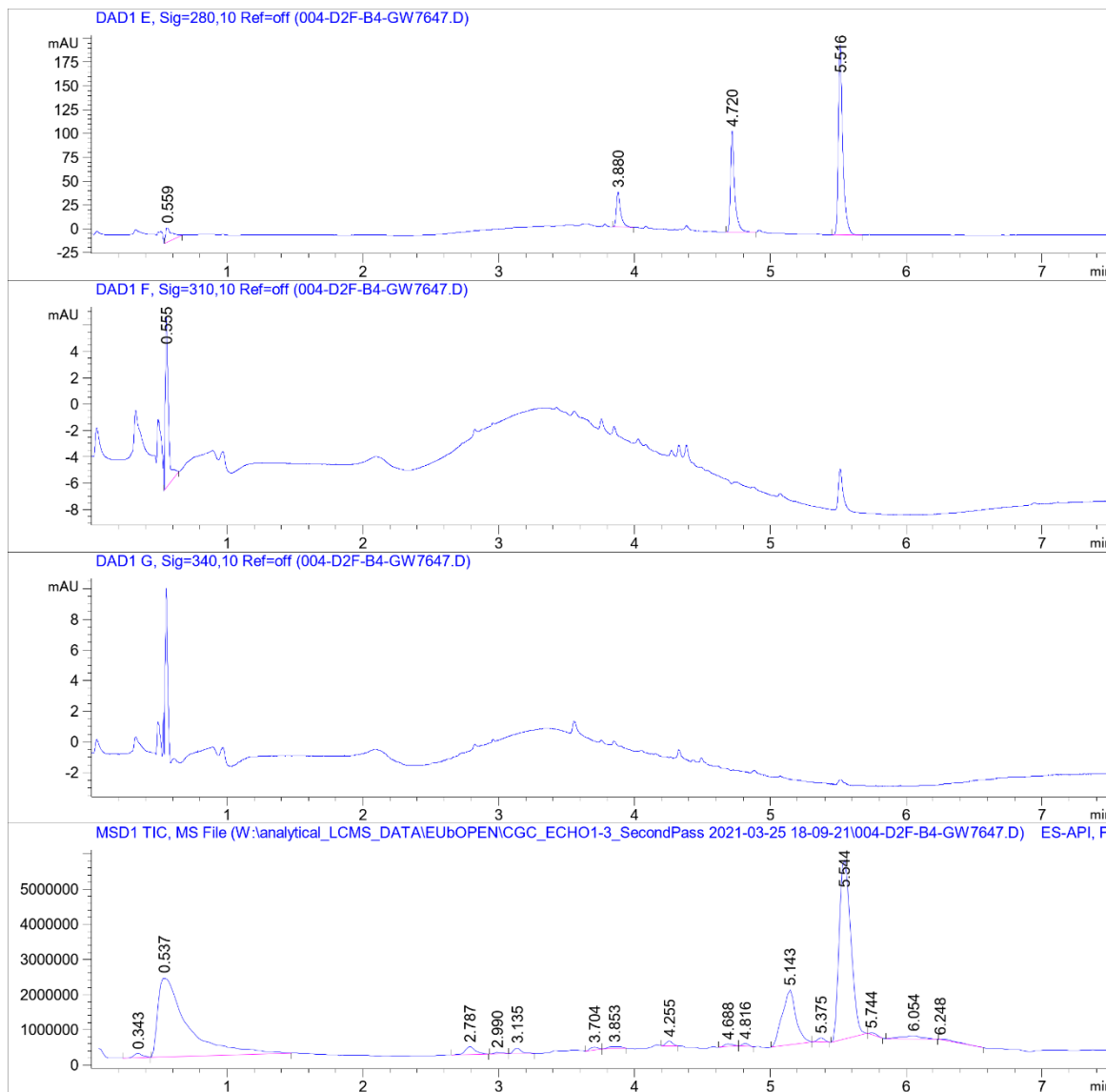
```
=====
Acq. Operator   : SYSTEM                      Seq. Line :    4
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2F-B4
Injection Date  : 3/25/2021 6:45:18 PM      Inj       :    1
                                           Inj Volume: Inj prog
Sequence File   : 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)
=====
```



# COMPOUND INFORMATION

Data File W:\analyti...OPEN\CGC\_ECH01-3\_SecondPass 2021-03-25 18-09-21\004-D2F-B4-GW7647.D

Sample Name: GW7647



# COMPOUND INFORMATION



Data File W:\analyti...OPEN\CGC\_ECH01-3\_SecondPass 2021-03-25 18-09-21\004-D2F-B4-GW7647.D

Sample Name: GW7647

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
-	-	0.343	531811	200.00 I 182.90 I 159.00 I 142.00 I
0.517	24	0.537	34150540	157.00 I
0.558	39	-	-	
-	-	2.787	1203455	217.10 I
-	-	2.990	187435	274.20 I
-	-	3.135	689244	378.30 I
-	-	3.704	311274	312.20 I 214.10 I 111.10 I
-	-	3.853	356953	316.30 I 298.20 I 288.20 I 282.30 I 252.20 I 225.20 I 200.00 I 159.00 I 111.10 I 110.10 I
-	-	4.255	445303	296.30 I
4.720	37	4.688	338247	254.30 I
-	-	4.816	230855	280.30 I
-	-	5.143	10786898	282.30 I
-	-	5.375	423401	489.40 I 282.30 I
5.516	241	5.544	29970410	503.40 I
-	-	5.744	218435	400.40 I 282.20 I
-	-	6.054	1001885	282.30 I

