

## GW9578

**CAS Registry No.:** 247923-29-1

**Formal Name:** 2-((4-(2-(3-(2,4-difluorophenyl)-1-heptylureido)ethyl)phenyl)thio)-2-methylpropanoic acid

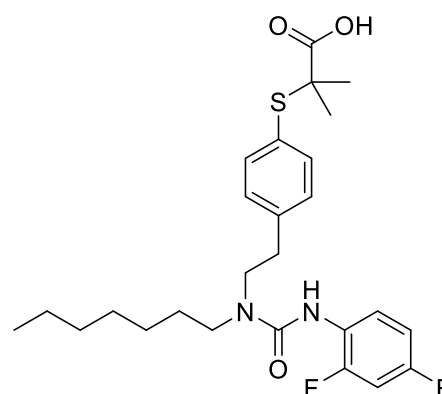
**EUbOPEN ID:** EUB0001142a

**Molecular Formula:** C<sub>26</sub>H<sub>34</sub>F<sub>2</sub>N<sub>2</sub>O<sub>3</sub>S

**Molecular Weight:** 492.63 g/mol

**Smiles:** CCCCCCCN(CCC1=CC=C(C=C1)SC(C)(C)C(=O)O)C(=O)NC2=C(C=C2)F

**Recommended concentration:** 1  $\mu$ M



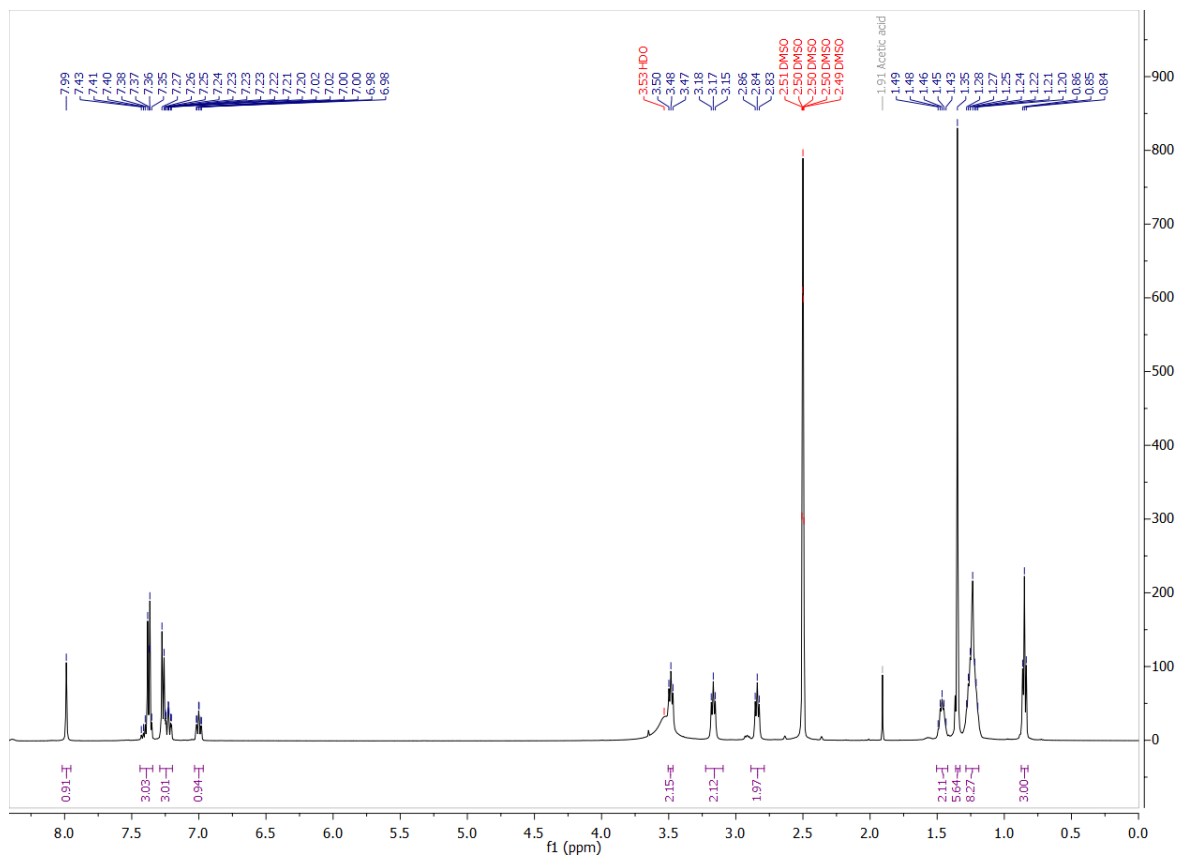
### Biological activity

		Type	IC <sub>50</sub> /EC <sub>50</sub> [ $\mu$ M]	Reference
Main NR target:	NR1C1 (PPAR $\alpha$ )	Agonist	0.05	<a href="https://doi.org/10.1021/jm9903601">https://doi.org/10.1021/jm9903601</a>
	NR1C3 (PPAR $\gamma$ )	Agonist	1	
NR off-target:	NR1C2 (PPAR $\delta$ )	Agonist	1	<a href="https://doi.org/10.1021/jm9903601">https://doi.org/10.1021/jm9903601</a>

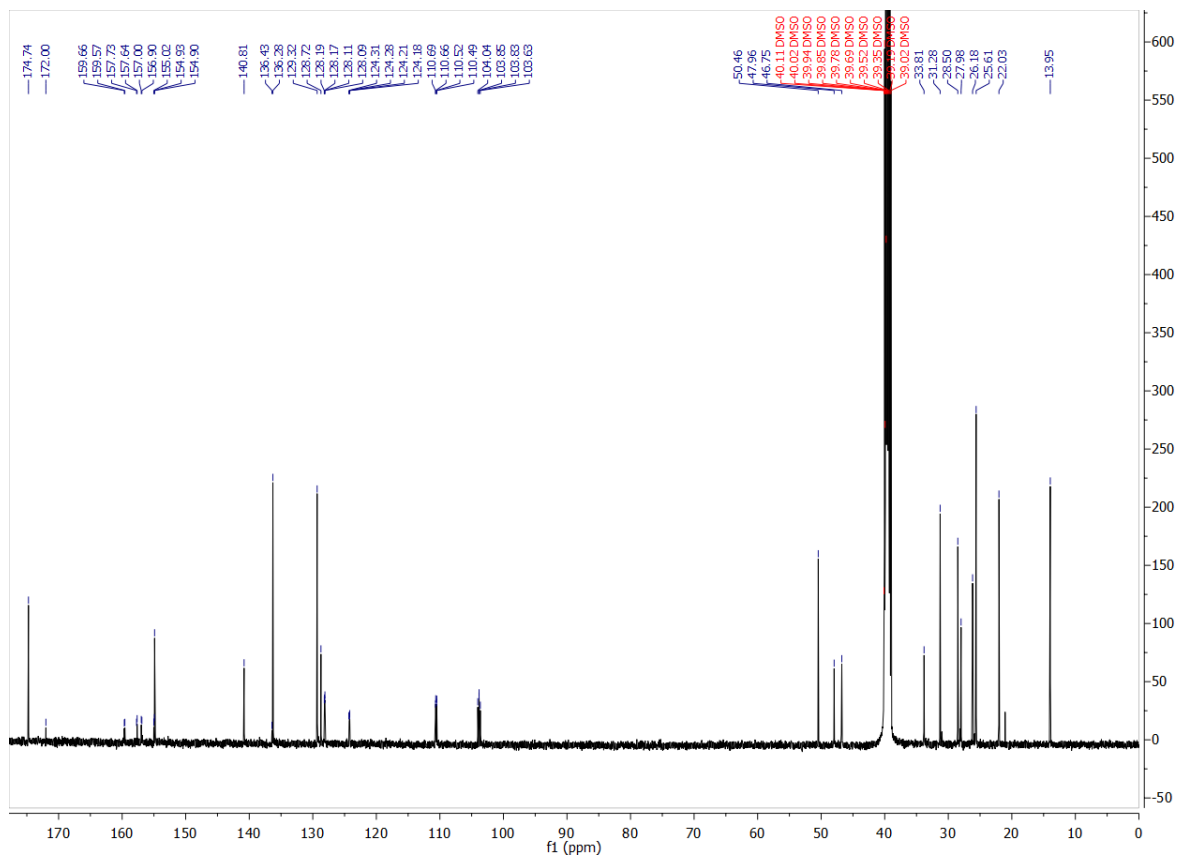
# COMPOUND INFORMATION

## Identity

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



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



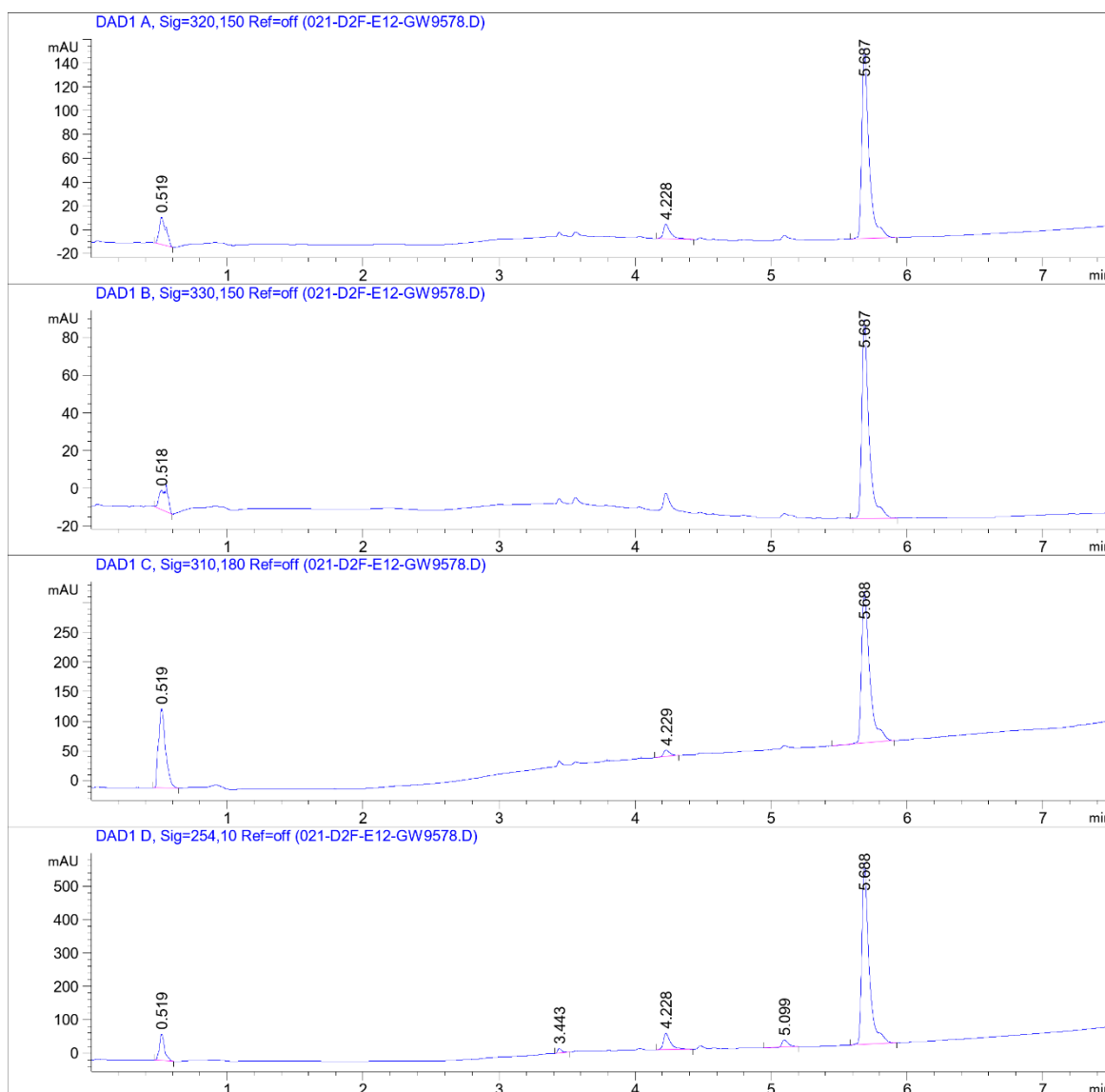
# COMPOUND INFORMATION

## Purity

Data File W:\analyti...PEN\CGC\_wave3\_1\_SecondPass 2023-01-19 20-16-18\021-D2F-E12-GW9578.D

Sample Name: GW9578

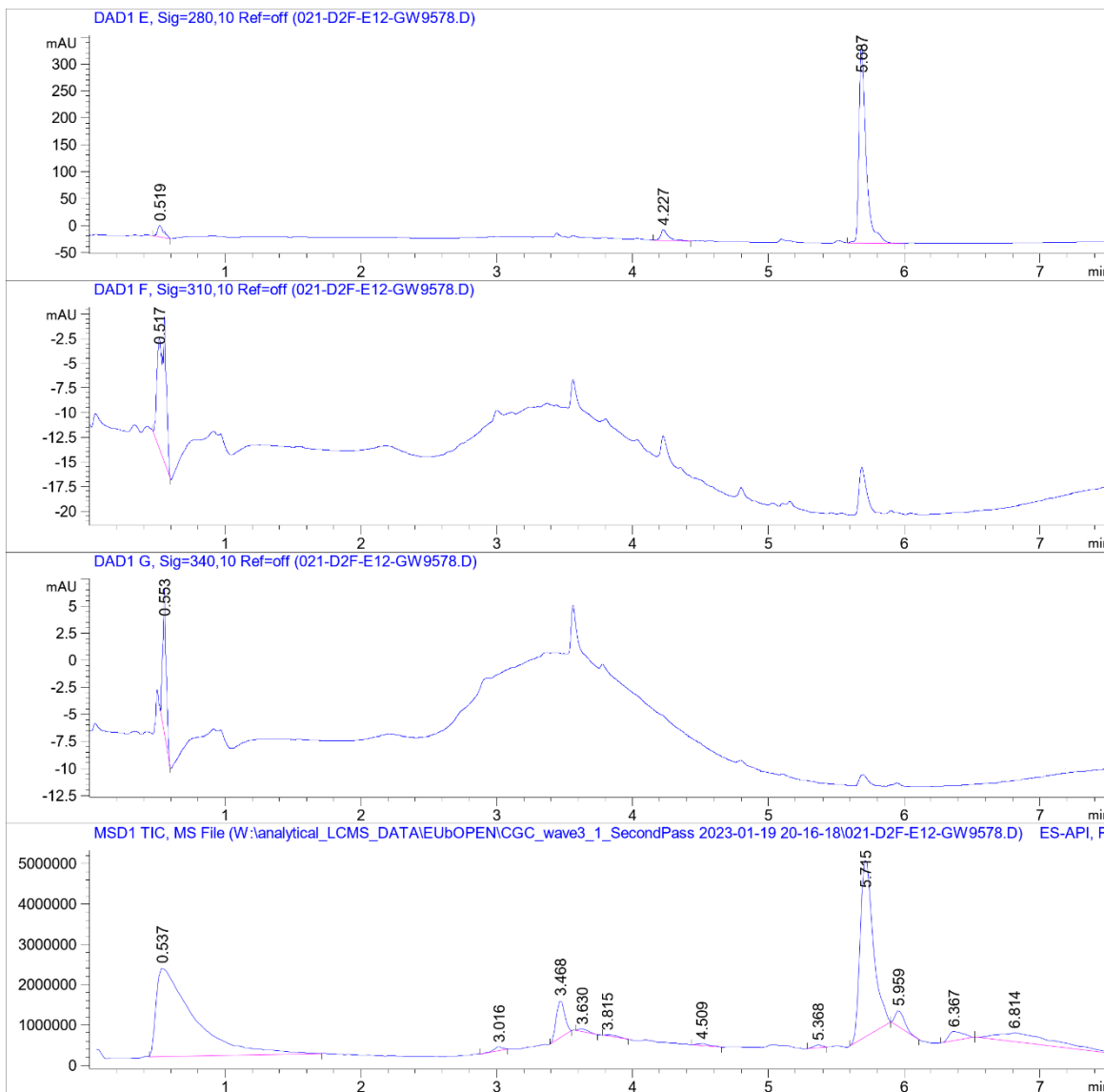
```
=====
Acq. Operator   : SYSTEM                      Seq. Line :   21
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2F-E12
Injection Date  : 1/20/2023 12:04:33 AM      Inj       :    1
                                           Inj Volume: Inj prog
Sequence File   : W:\analytical_LCMS_DATA\EUBOPEN\CGC_wave3_1_SecondPass 2023-01-19 20-16-18
                                           \CGC_wave3_1_SecondPass.S
Method          : W:\analytical_LCMS_DATA\EUBOPEN\CGC_wave3_1_SecondPass 2023-01-19 20-16-18
                                           \CGL_SECONDPASS_NONPOLCOMP_VIAL2+4_20210323.M (Sequence Method)
Last changed    : 7/18/2022 10:07:35 AM 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...PEN\CGC\_wave3\_1\_SecondPass 2023-01-19 20-16-18\021-D2F-E12-GW9578.D

Sample Name: GW9578



# COMPOUND INFORMATION

Data File W:\analyti...PEN\CGC\_wave3\_1\_SecondPass 2023-01-19 20-16-18\021-D2F-E12-GW9578.D

Sample Name: GW9578

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
0.519	80	0.537	42307164	157.00 I
-	-	3.016	375098	239.00 I 217.00 I 170.80 I
-	-	3.468	3880490	338.20 I
-	-	3.630	335096	170.80 I
-	-	3.815	304643	170.80 I
4.228	45	-	-	
-	-	4.509	313730	510.30 I 170.80 I
-	-	5.368	263254	510.30 I 348.20 I 280.20 I 228.20 I 137.10 I
5.687	584	5.715	29392894	515.20 I 493.20 I
-	-	5.959	1827537	282.20 I
-	-	6.367	1661544	284.20 I 282.20 I 137.10 I
-	-	6.814	6881839	282.20 I 137.10 I

