

## GW590735

**CAS Registry No.:** 622402-22-6

**Formal Name:** 2-methyl-2-(4-((4-methyl-2-(4-(trifluoromethyl)phenyl)thiazole-5-carboxamido)methyl)phenoxy)propanoic acid

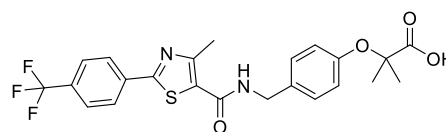
**EUBOPEN ID:** EUB0001141a

**Molecular Formula:** C<sub>23</sub>H<sub>21</sub>F<sub>3</sub>N<sub>2</sub>O<sub>4</sub>S

**Molecular Weight:** 478.49 g/mol

**Smiles:**  
CC1=C(SC(=N1)C2=CC=C(C=C2)C(F)(F)F)C(=O)NCC3=CC=C(C=C3)OC(C)(C)C(=O)O

**Recommended concentration:** 1 μM

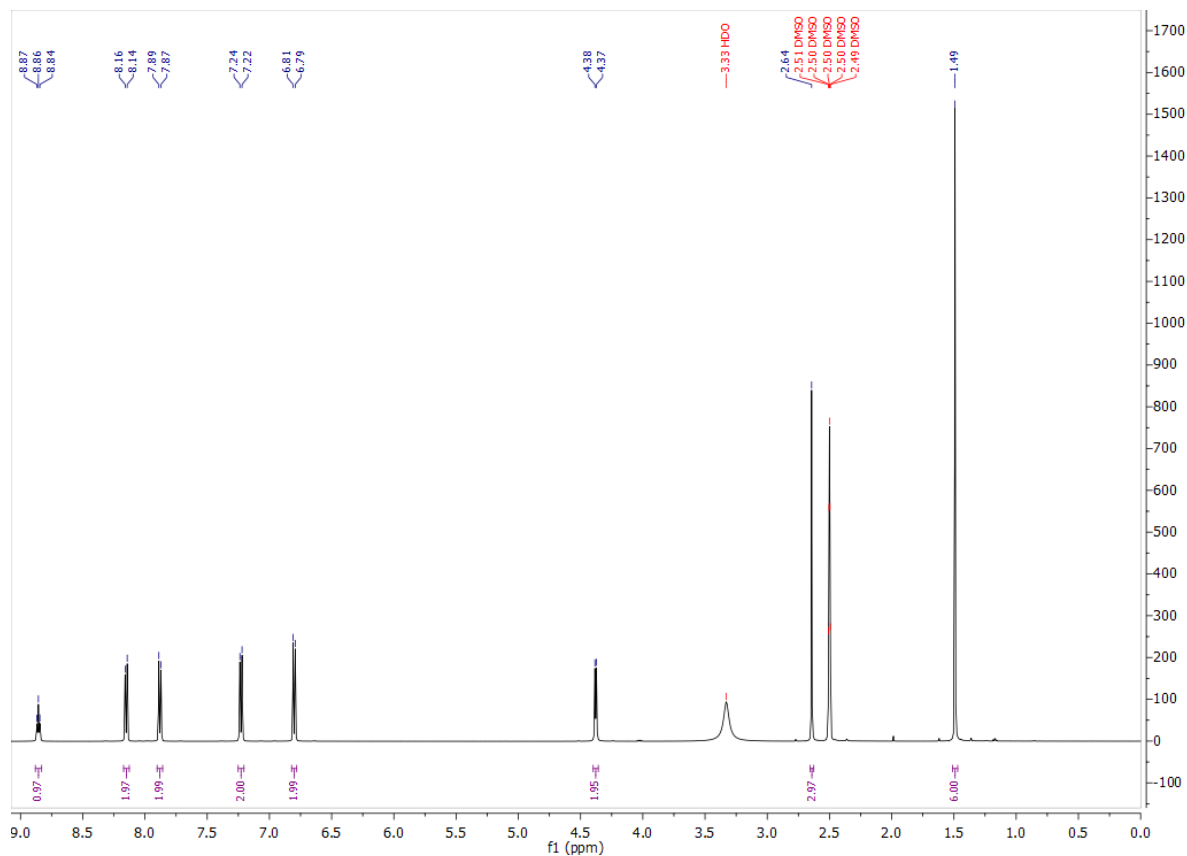


### Biological activity

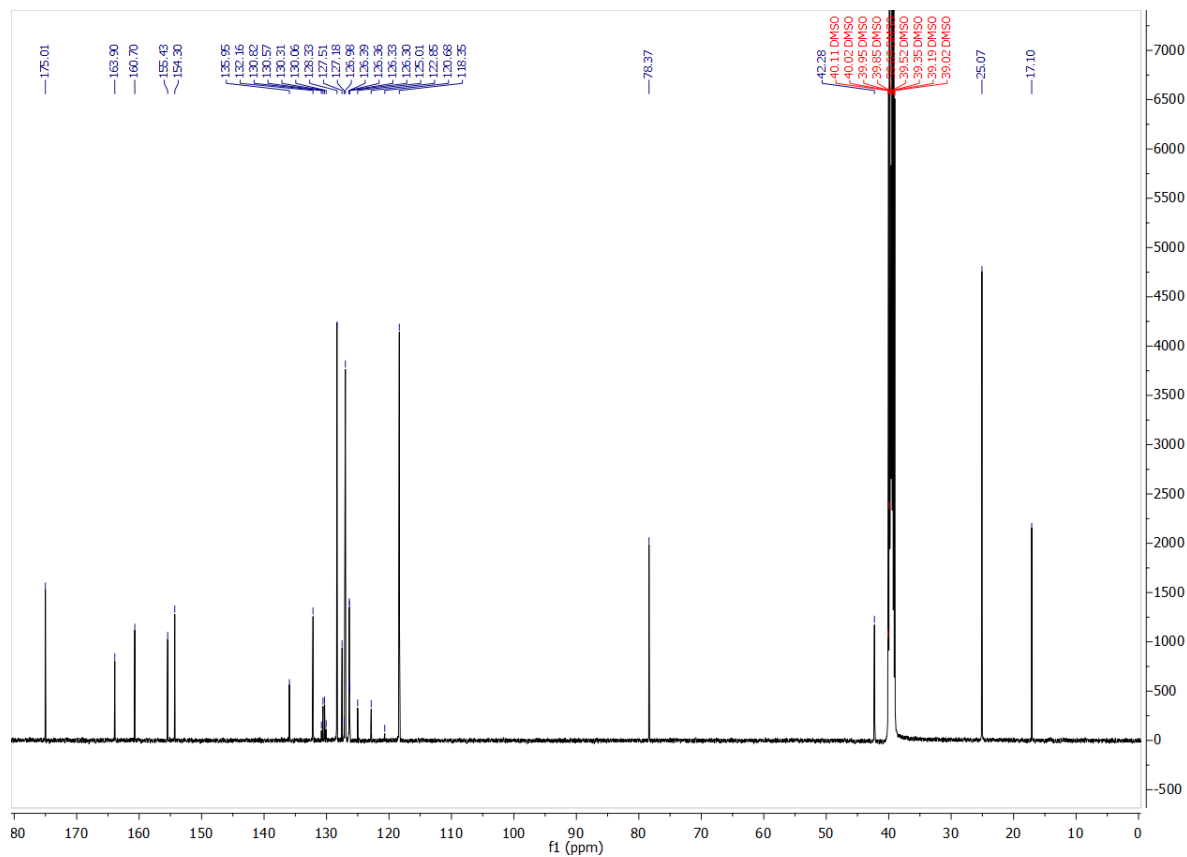
|                 |               | Type    | IC <sub>50</sub> /EC <sub>50</sub><br>[μM] | Reference  |
|-----------------|---------------|---------|--|--|
| Main NR target: | NR1C1 (PPARα) | Agonist | 0.004                                      | <a href="https://doi.org/10.1021/jm058056x">https://doi.org/10.1021/jm058056x</a> ,<br><a href="https://doi.org/10.1016/j.bmcl.2008.09.094">https://doi.org/10.1016/j.bmcl.2008.09.094</a> |
|                 | NR1C2 (PPARδ) | Agonist | 0.15                                       | inhouse  |
| NR off-target:  |               |         |  |  |

## Identity

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



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



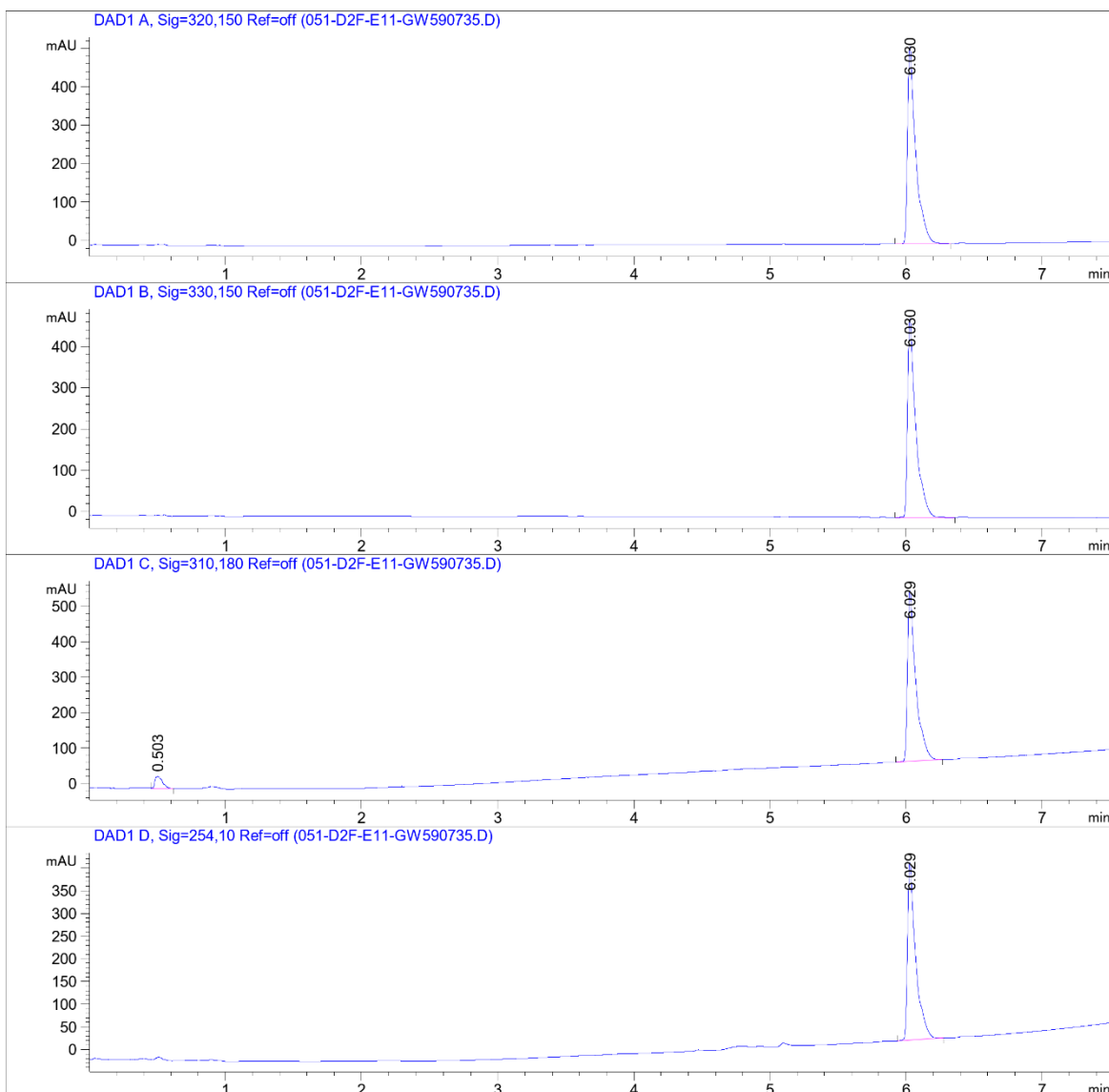
# COMPOUND INFORMATION

## Purity

Data File W:\analyti...\N\CGC\_wave3\_1\_FirstPassB 2023-01-04 18-28-02\051-D2F-E11-GW590735.D

Sample Name: GW590735

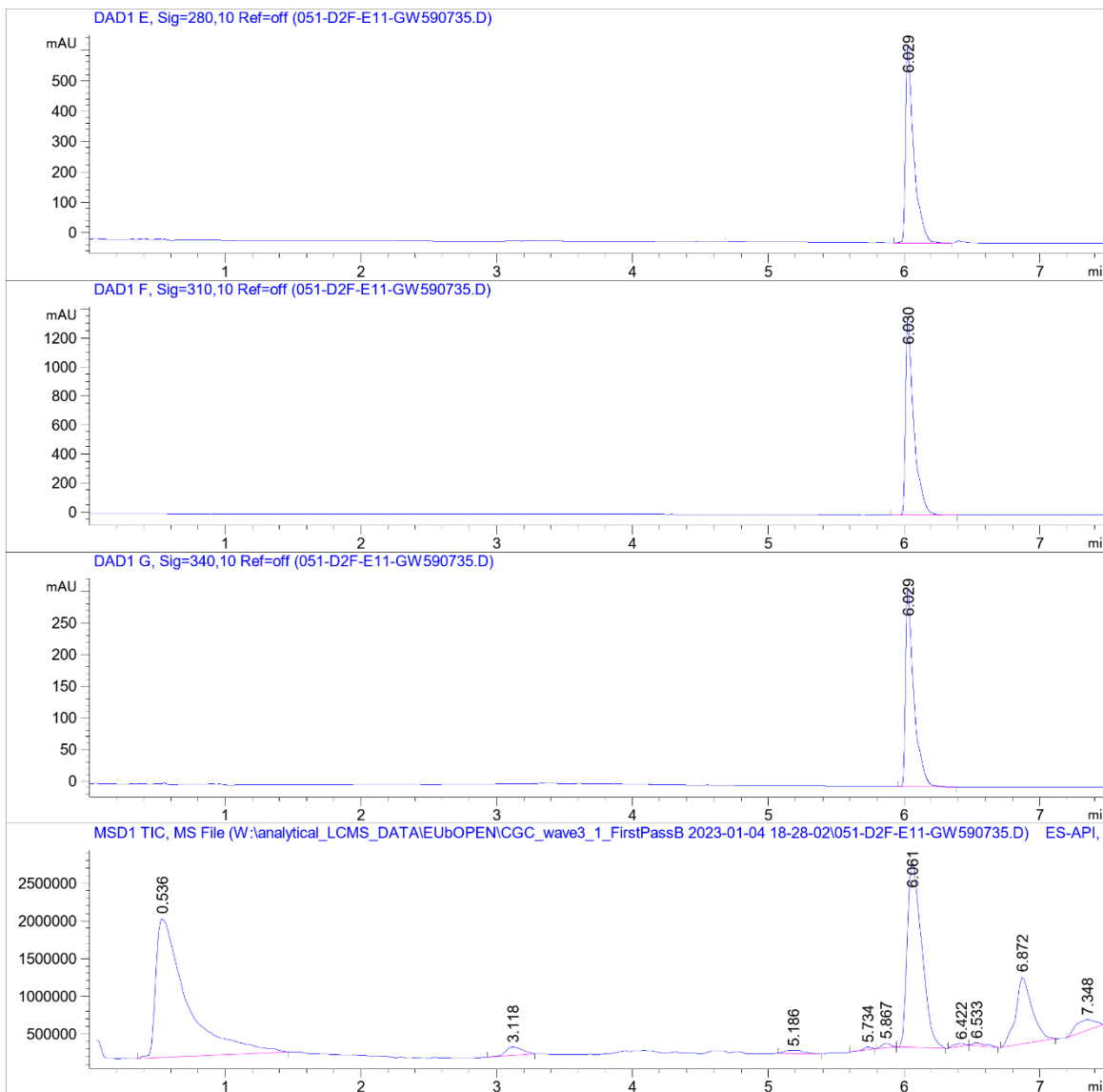
```
=====
Acq. Operator   : SYSTEM                      Seq. Line :   51
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2F-E11
Injection Date  : 1/5/2023 3:43:44 AM         Inj       :    1
                                           Inj Volume: Inj prog
Sequence File   : 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
=====
```



# COMPOUND INFORMATION

Data File W:\analyti...N\CGC\_wave3\_1\_FirstPassB 2023-01-04 18-28-02\051-D2F-E11-GW590735.D

Sample Name: GW590735



# COMPOUND INFORMATION

Data File W:\analyti...\CGC\_wave3\_1\_FirstPassB 2023-01-04 18-28-02\051-D2F-E11-GW590735.D

Sample Name: GW590735

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

Spectra from peak tops.

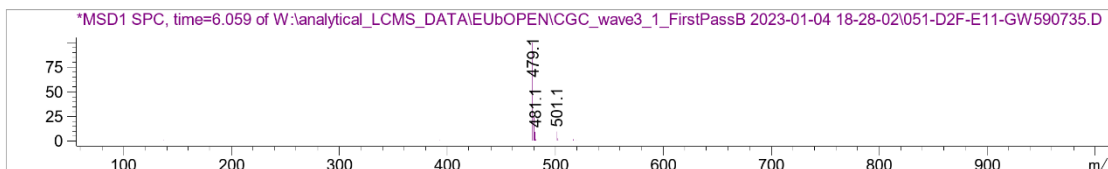
Noise Cutoff: 1000 counts.

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               | 29029588 | 157.00 I                                     |
| -                   | -       | 3.118               | 968117   | 239.10 I<br>217.10 I                         |
| -                   | -       | 5.186               | 435414   | 510.40 I<br>170.90 I<br>137.10 I             |
| -                   | -       | 5.734               | 149111   | 280.20 I                                     |
| -                   | -       | 5.867               | 285303   | 318.20 I<br>296.20 I                         |
| 6.030               | 2127    | 6.061               | 18284772 | 479.10 I                                     |
| -                   | -       | 6.422               | 227439   | 350.20 I<br>282.20 I<br>254.20 I<br>137.10 I |
| -                   | -       | 6.533               | 278988   | 280.20 I                                     |
| -                   | -       | 6.872               | 7389712  | 282.20 I                                     |
| -                   | -       | 7.348               | 1466862  | 400.30 I<br>282.30 I                         |



# COMPOUND INFORMATION

## Biological activity

**GW590735**  
**PPAR $\delta$  - EC<sub>50</sub> 0.15  $\pm$  0.05  $\mu$ M**  
**26  $\pm$  2 fold activation**

