

## AC-261066

**CAS Registry No.:** 870773-76-5

**Formal Name:** 4-(4-(2-butoxyethoxy)-5-methylthiazol-2-yl)-2-fluorobenzoic acid

**EUBOPEN ID:** EUB0000835a

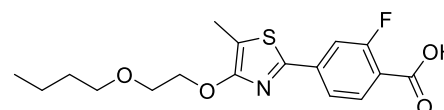
**Molecular Formula:** C<sub>17</sub>H<sub>20</sub>FNO<sub>4</sub>S

**Molecular Weight:** 353.41 g/mol

**Smiles:** CCCCOCCOC1=C(SC(=N1)C2=C(C(=C(C=C2)C(=O)O)F)C

**Purity:** 100 %

**Recommended concentration:** 1 μM

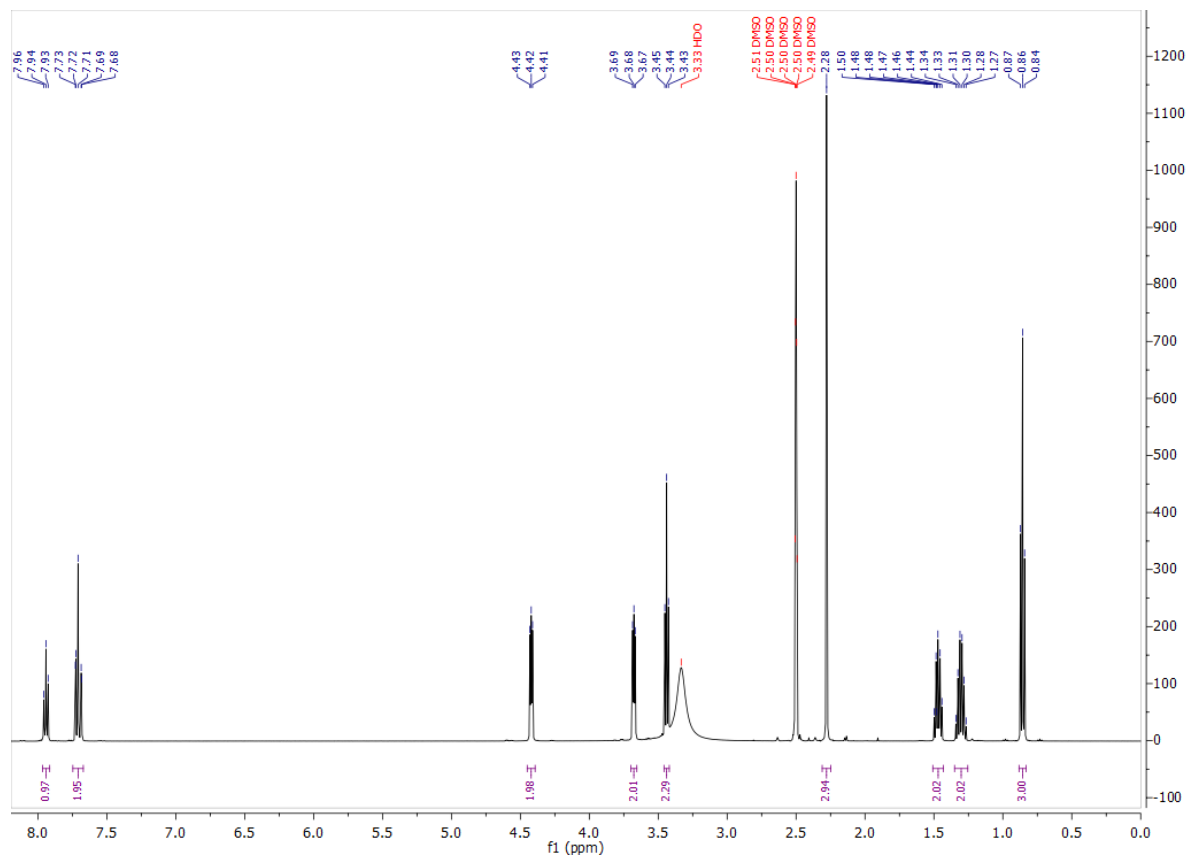


### Biological activity

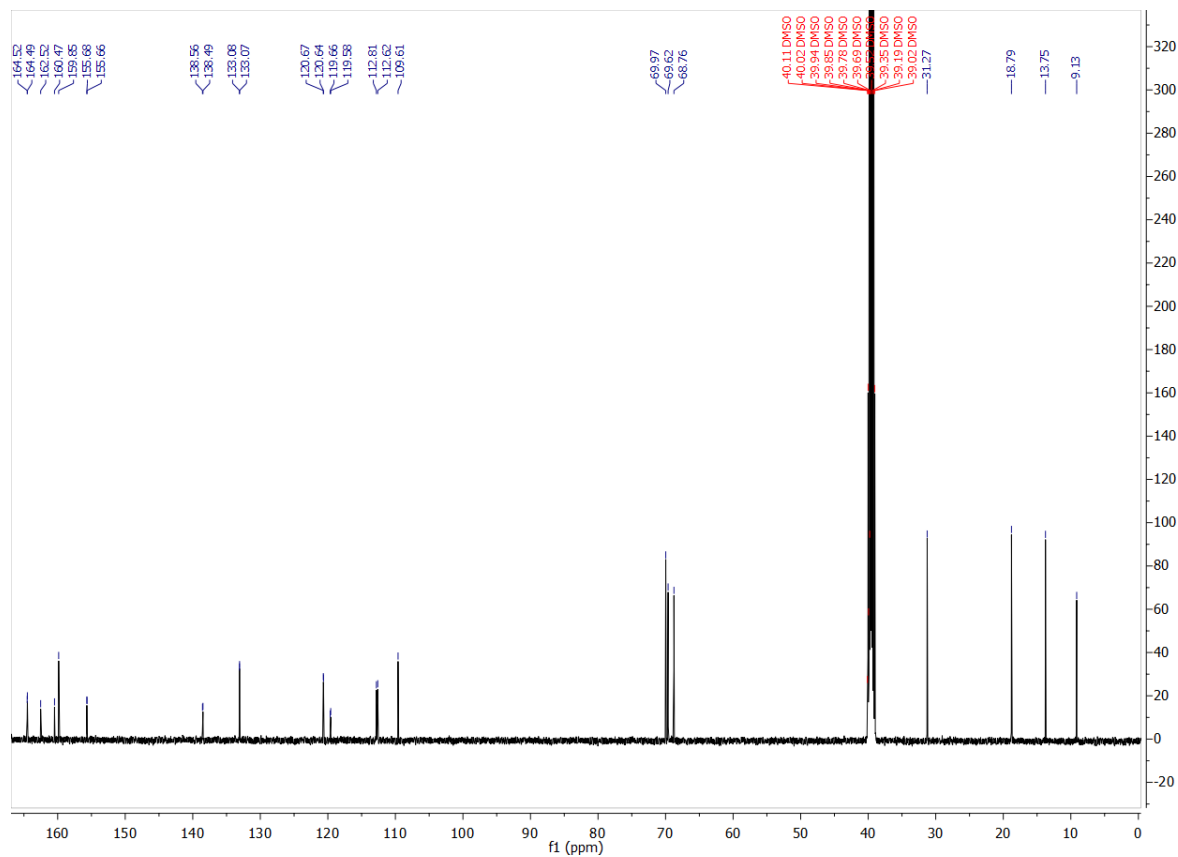
		Type	IC <sub>50</sub> /EC <sub>50</sub> [μM]	Reference
Main NR target:	NR1B1 (RARα)	Agonist	0.6	<a href="https://doi.org/10.1021/jm801532e">https://doi.org/10.1021/jm801532e</a> , <a href="https://doi.org/10.1021/jm050891r">https://doi.org/10.1021/jm050891r</a>
	NR1B2 (RARβ)	Agonist	0.010	
	NR1B3 (RARγ)	Agonist	0.5	
NR off-target:	NR2B1 (RXRα)	Agonist	26-fold act.	inhouse

## Identity

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



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



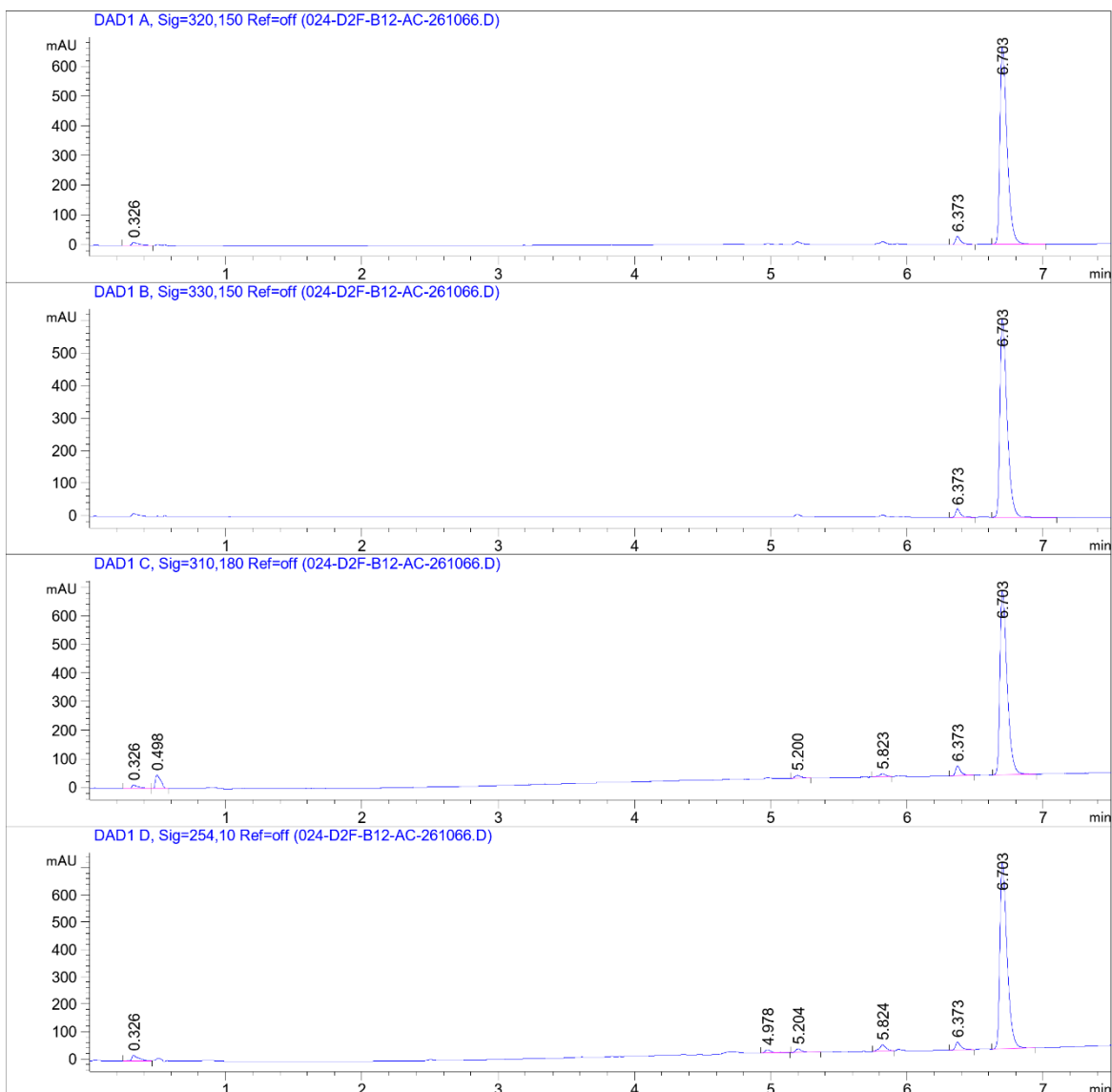
# COMPOUND INFORMATION

## Purity

Data File W:\analyti...\CGC\_wave2\_4\_FirstPassB 2022-02-18 17-58-18\024-D2F-B12-AC-261066.D

Sample Name: AC-261066

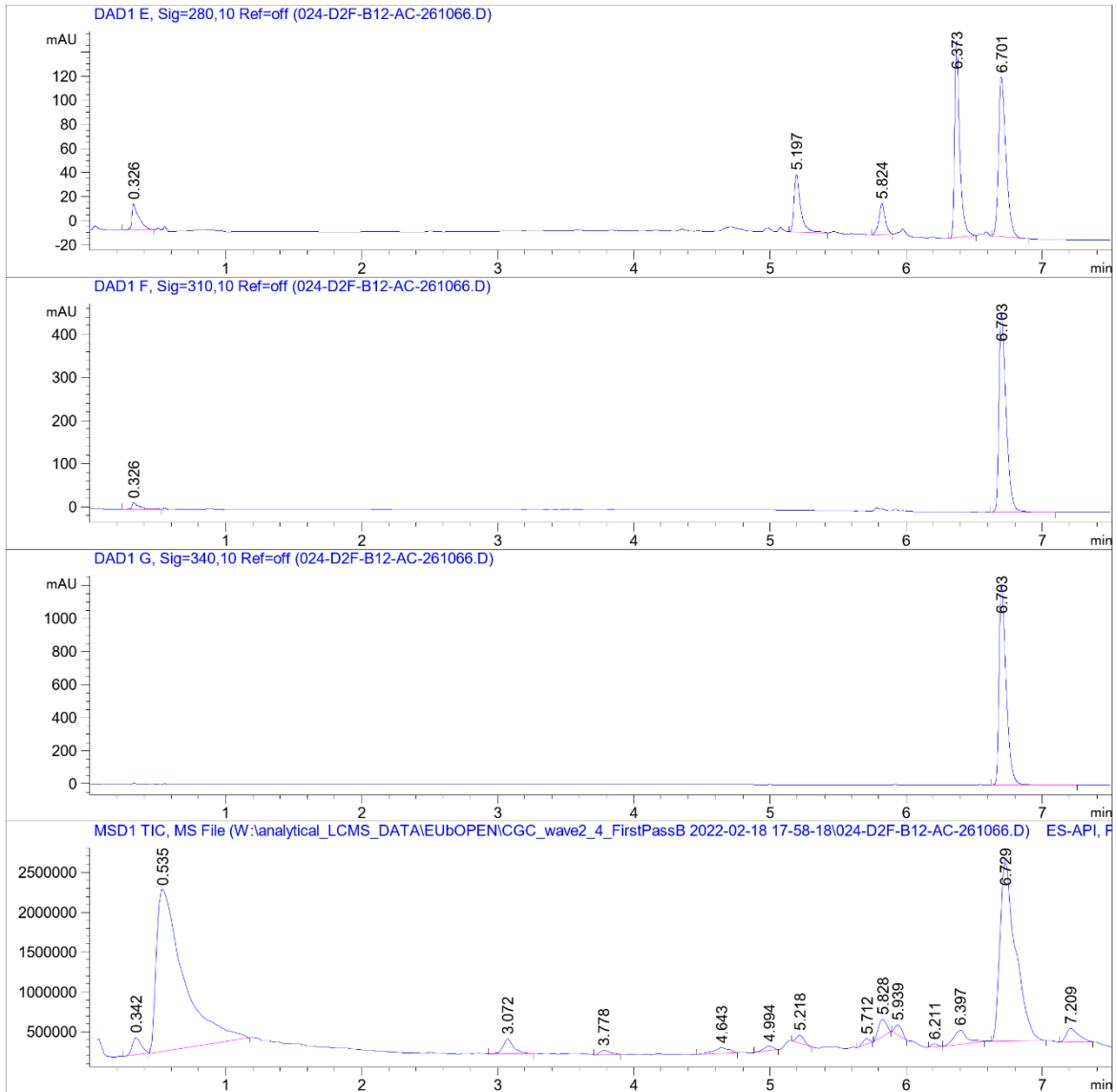
```
=====
Acq. Operator   : SYSTEM                      Seq. Line :   24
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2F-B12
Injection Date  : 2/18/2022 10:15:29 PM      Inj       :    1
                                           Inj Volume: Inj prog
Sequence File   : W:\analytical_LCMS_DATA\EUBOPEN\CGC_wave2_4_FirstPassB 2022-02-18 17-58-18
                  \CGC_wave2_4_FirstPassB.S
Method          : W:\analytical_LCMS_DATA\EUBOPEN\CGC_wave2_4_FirstPassB 2022-02-18 17-58-18
                  \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...\CGC\_wave2\_4\_FirstPassB 2022-02-18 17-58-18\024-D2F-B12-AC-261066.D

Sample Name: AC-261066



# COMPOUND INFORMATION



Data File W:\analyti...\CGC\_wave2\_4\_FirstPassB 2022-02-18 17-58-18\024-D2F-B12-AC-261066.D

Sample Name: AC-261066

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
0.326	38	0.342	972044	183.00 I 158.90 I 141.90 I
-	-	0.535	28038024	157.00 I
-	-	3.072	1038603	239.00 I 217.00 I
-	-	3.778	295049	274.20 I
-	-	4.643	553328	332.20 I
-	-	4.994	278035	350.00 I 328.10 I
-	-	5.218	395665	316.20 I 298.20 I
-	-	5.712	208873	280.20 I
-	-	5.828	887903	543.20 I 318.20 I 296.20 I
-	-	5.939	467711	318.20 I 296.20 I 282.20 I 280.20 I
-	-	6.211	132407	228.10 I
6.373	72	6.397	1223767	350.20 I 282.20 I 254.20 I 243.00 I
6.703	2412	6.729	18031048	354.10 I
-	-	7.209	1092900	284.20 I 282.20 I

