

## GW4064

**CAS Registry No.:** 278779-30-9

**Formal Name:** (E)-3-(2-chloro-4-((3-(2,6-dichlorophenyl)-5-isopropylisoxazol-4-yl)methoxy)styryl)benzoic acid

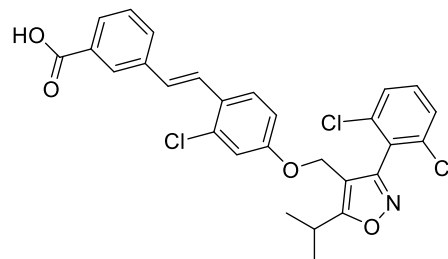
**EUBOPEN ID:** EUB0000184b

**Molecular Formula:** C<sub>28</sub>H<sub>22</sub>Cl<sub>3</sub>NO<sub>4</sub>

**Molecular Weight:** 542.84 g/mol

**Smiles:** O=C(C1=CC=CC(/C=C/C2=CC=C(C=C2Cl)OCC3=C(ON=C3C4=C(C=CC=C4Cl)Cl)C(C)C)=C1)O

**Recommended concentration:** 1 μM



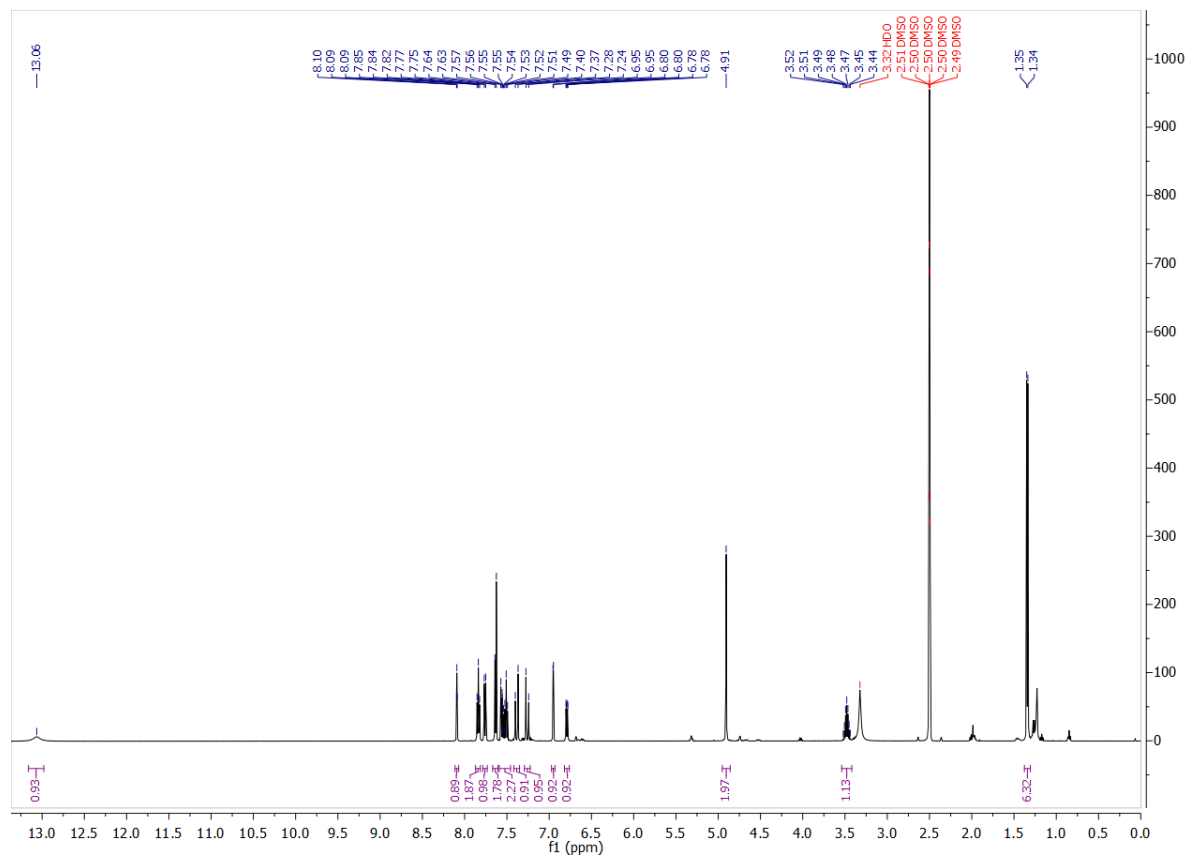
### Biological activity

		Type	IC <sub>50</sub> /EC <sub>50</sub> [μM]	Reference
Main NR target:	NR1H4 (FXR)	Agonist	0.37	inhouse
NR off-target:				

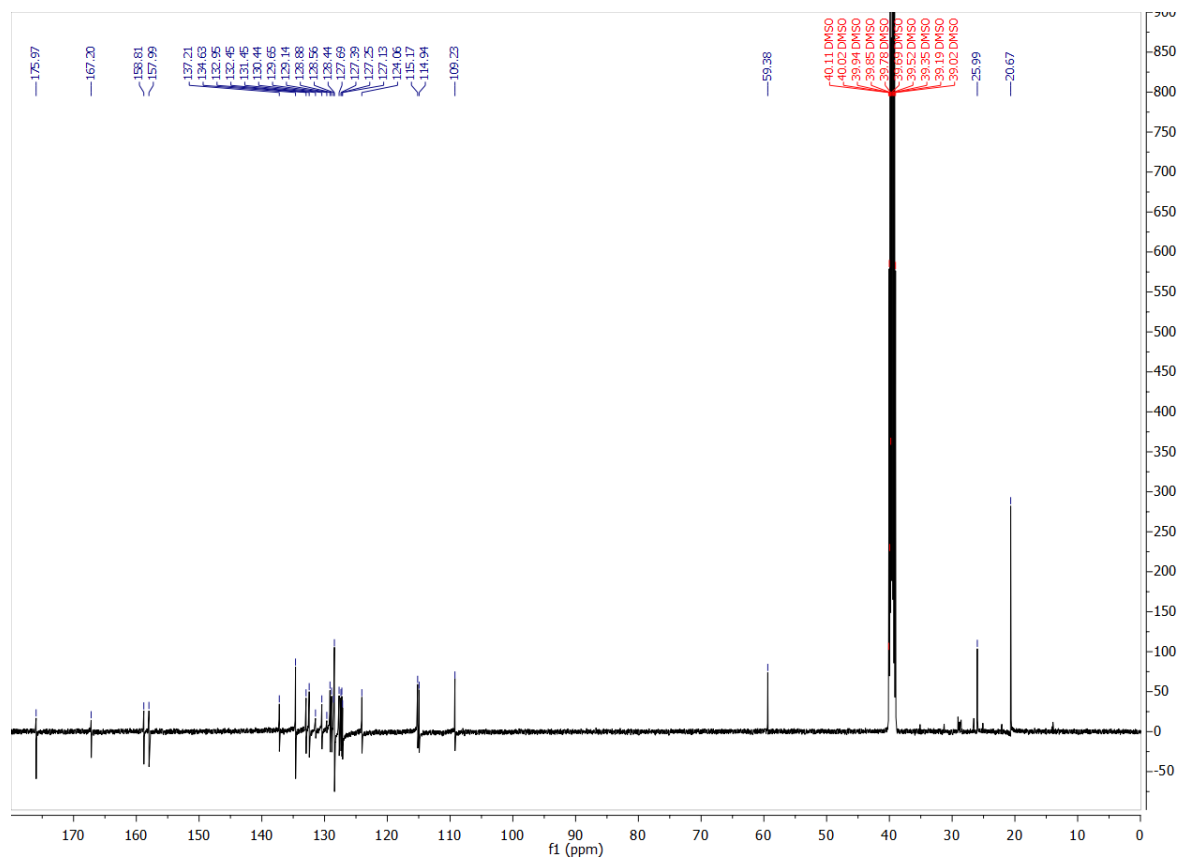
# COMPOUND INFORMATION

## Identity

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



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



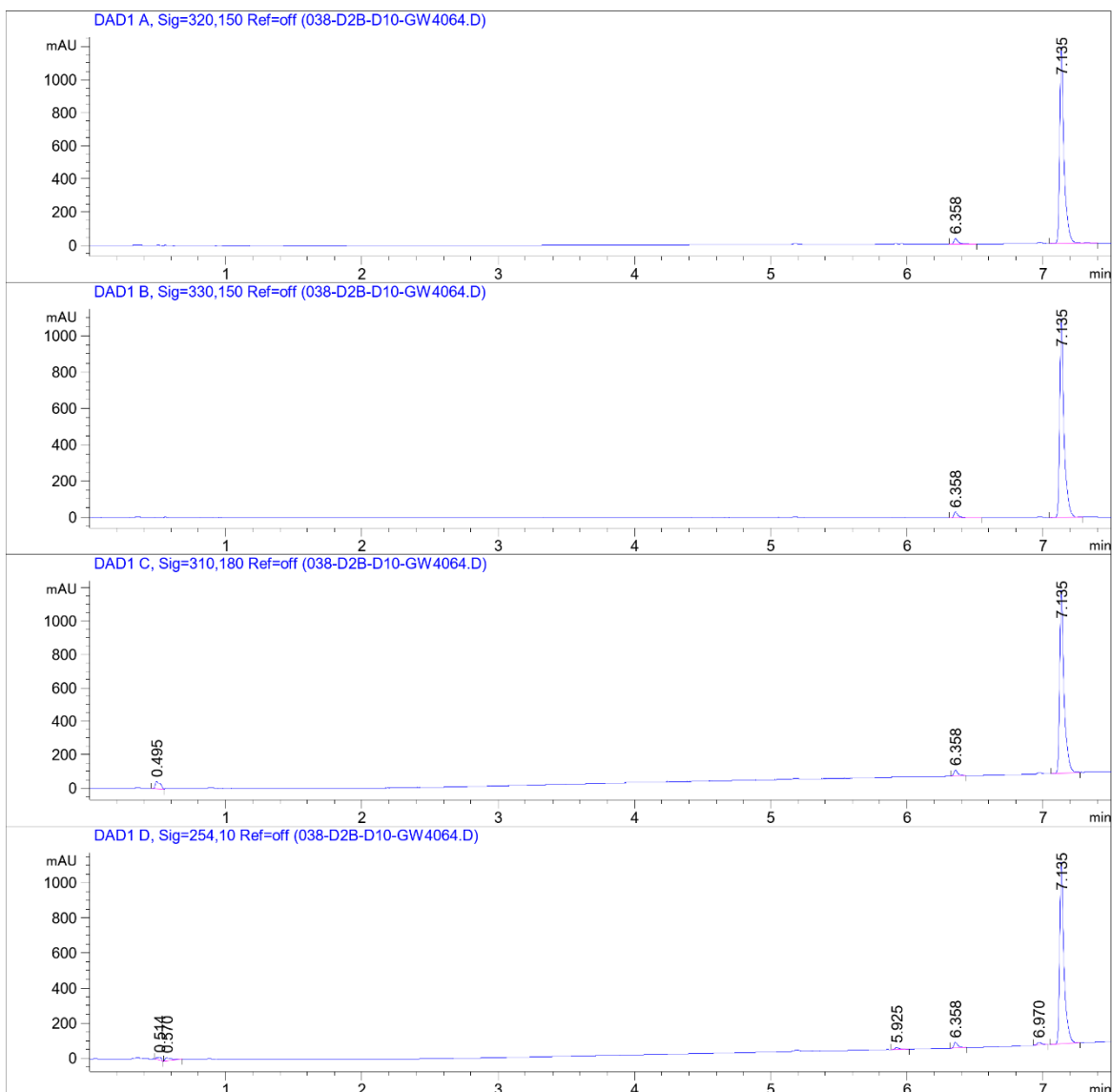
# COMPOUND INFORMATION

## Purity

Data File W:\analyti...OPEN\CGC\_ECH01-3\_FirstPass 2021-03-20 13-21-54\038-D2B-D10-GW4064.D

Sample Name: GW4064

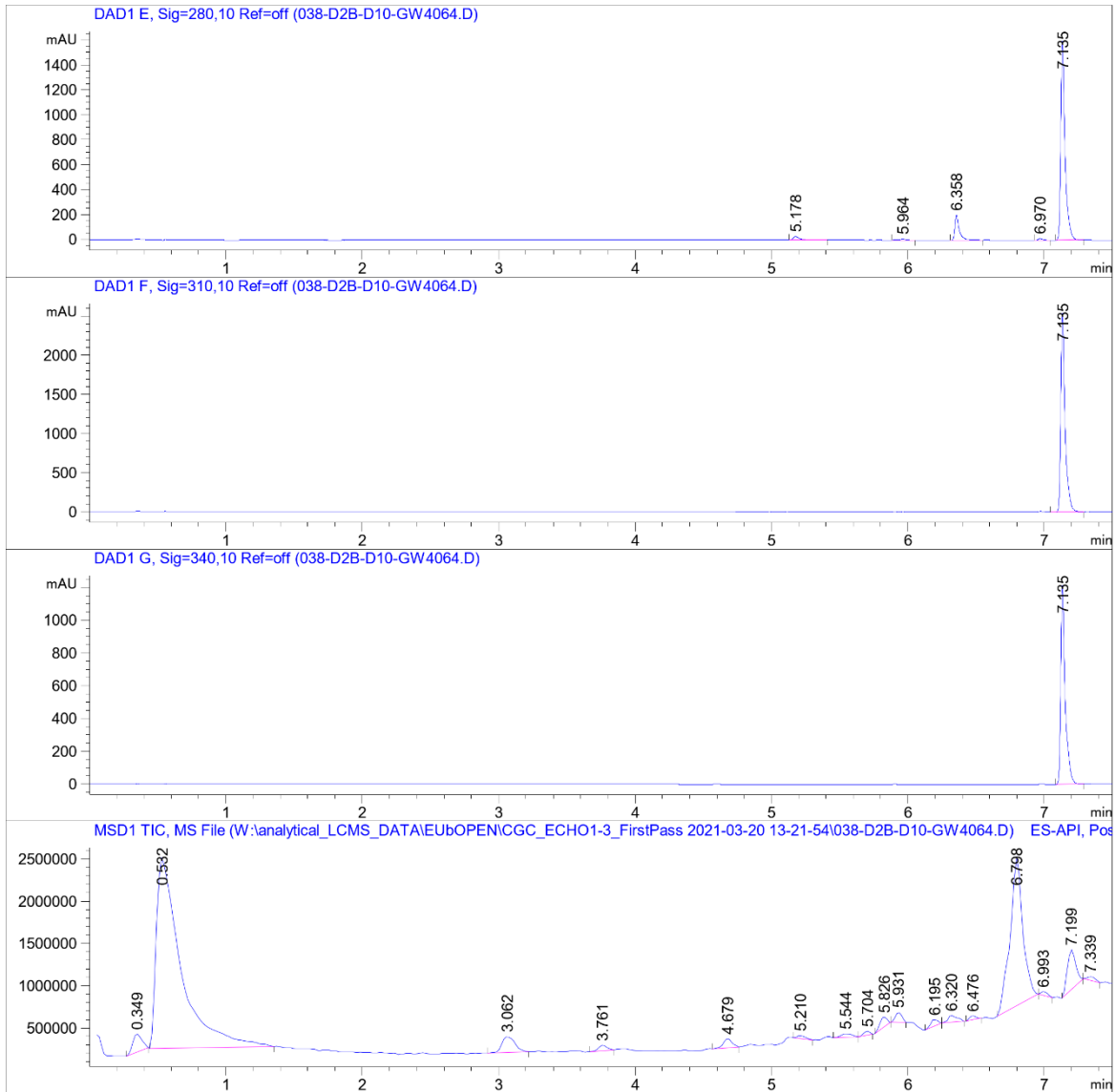
```
=====
Acq. Operator   : SYSTEM                      Seq. Line :   38
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2B-D10
Injection Date  : 3/20/2021 8:15:40 PM       Inj       :    1
                                           Inj Volume: Inj prog
Sequence File   : W:\analytical_LCMS_DATA\EUBOPEN\CGC_ECH01-3_FirstPass 2021-03-20 13-21-54
                                           \CGC_ECH01-3_FirstPass.S
Method          : W:\analytical_LCMS_DATA\EUBOPEN\CGC_ECH01-3_FirstPass 2021-03-20 13-21-54
                                           \CGL_FIRSTPASS_GENERALMETHOD_VIAL3+4_20210319.M (Sequence Method)
Last changed    : 3/19/2021 5:35:24 PM by SYSTEM
Method Info     : CGL wellplate, 0.5 uL of 10 mM DMSO, general method
=====
```



# COMPOUND INFORMATION

Data File W:\analyti...OPEN\CGC\_ECHO1-3\_FirstPass 2021-03-20 13-21-54\038-D2B-D10-GW4064.D

Sample Name: GW4064



# COMPOUND INFORMATION

Data File W:\analyti...OPEN\CGC\_ECHO1-3\_FirstPass 2021-03-20 13-21-54\038-D2B-D10-GW4064.D

Sample Name: GW4064

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

Spectra from peak tops.

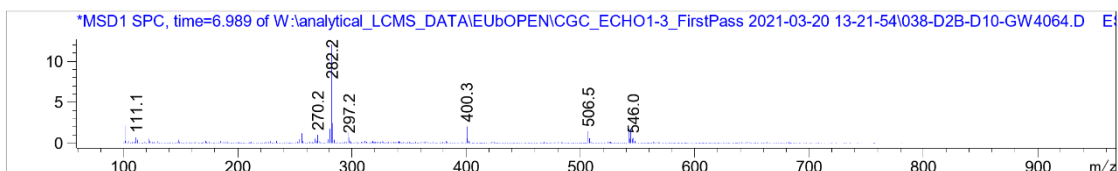
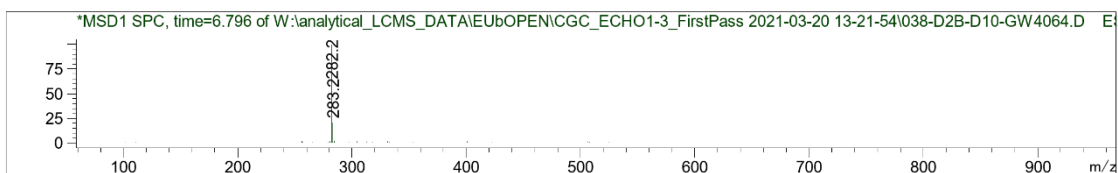
Noise Cutoff: 1000 counts.

Reportable Ion Abundance: > 50%.

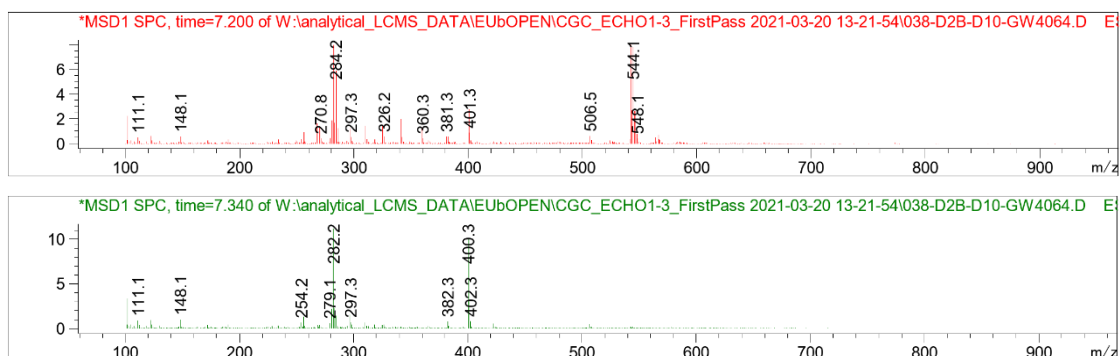
LC Signal: DAD1 A, Sig=320,150 Ref=off

Peak matching window: 0.1 min

Retention Time (LC)	LC Area	Retention Time (MS)	MS Area	Mol. Weight or Ion
-	-	0.349	1009973	157.90 I 130.00 I
-	-	0.532	28215774	157.00 I
-	-	3.062	1250510	217.10 I
-	-	3.761	285437	274.20 I
-	-	4.679	482301	326.30 I
-	-	5.210	153077	316.20 I 102.20 I
-	-	5.544	237946	326.20 I 280.20 I 102.20 I
-	-	5.704	144632	280.20 I
-	-	5.826	437411	296.20 I
-	-	5.931	393297	296.20 I 294.20 I 280.20 I
-	-	6.195	295054	280.20 I 228.20 I
6.358	75	6.320	387414	254.20 I
-	-	6.476	165237	280.20 I
-	-	6.798	11393991	282.20 I
-	-	6.993	153786	282.20 I
7.135	2622	7.199	2005478	544.10 I 542.10 I 284.20 I 282.20 I
-	-	7.339	184484	400.30 I 282.20 I



# COMPOUND INFORMATION



## Biological activity

**GW4064**  
**FXR - EC<sub>50</sub> 0.37 ± 0.03 μM**  
**366 ± 11 fold activation**

