

## CP775146

**CAS Registry No.:** 702680-17-9

**Formal Name:** 2-(3-(1-(2-(4-isopropylphenyl)acetyl)piperidin-3-yl)phenoxy)-2-methylpropanoic acid

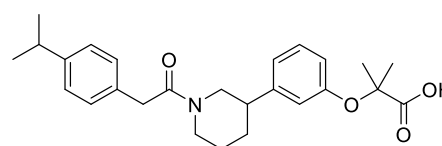
**EUBOPEN ID:** EUB0000581a

**Molecular Formula:** C<sub>26</sub>H<sub>33</sub>NO<sub>4</sub>

**Molecular Weight:** 423.55 g/mol

**Smiles:**  
CC(C)C1=CC=C(C=C1)CC(=O)N2CCCC(C2)C3=CC(=CC=C3)OC(C)(C)C(=O)O

**Recommended concentration:** 1 μM



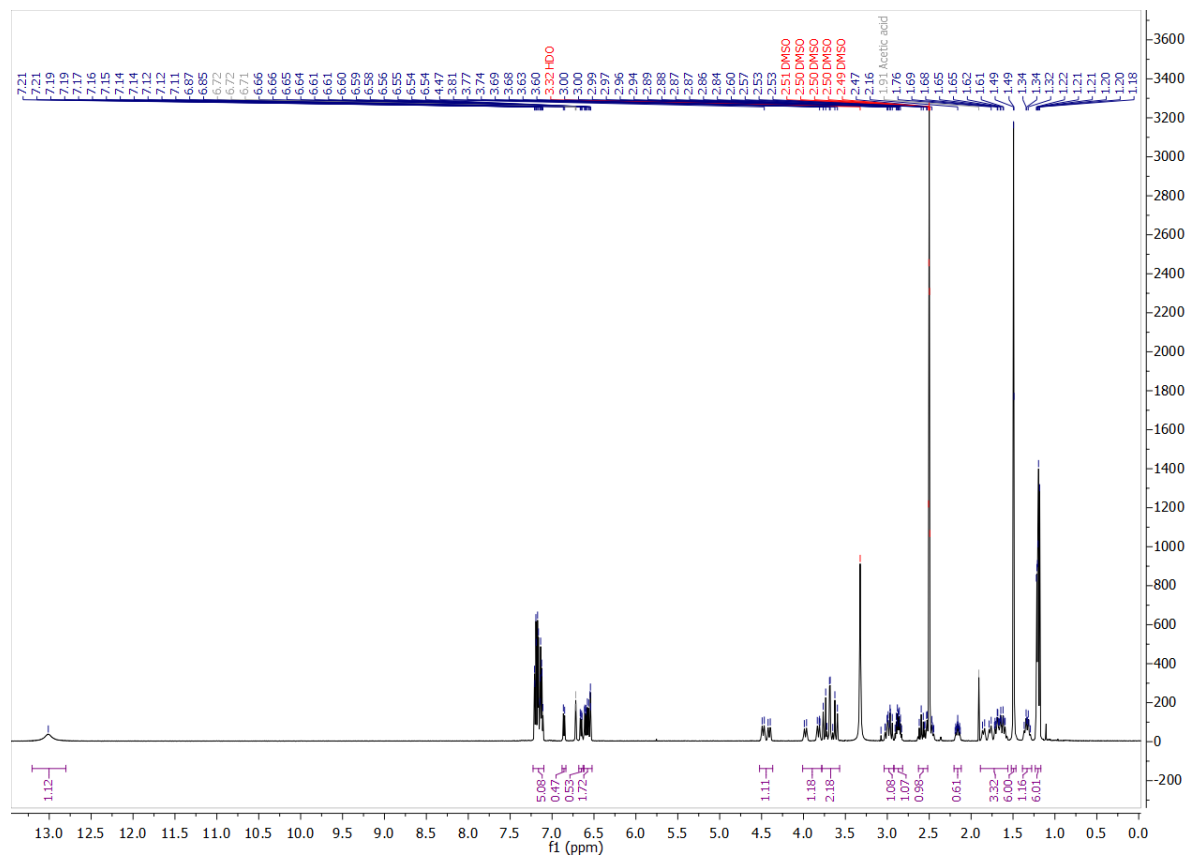
### Biological activity

		Type	IC <sub>50</sub> /EC <sub>50</sub> [μM]	Reference
Main NR target:	NR1C1 (PPARα)	Agonist	0.06	<a href="https://doi.org/10.1124/mol.108.051656">https://doi.org/10.1124/mol.108.051656</a>
NR off-target:				

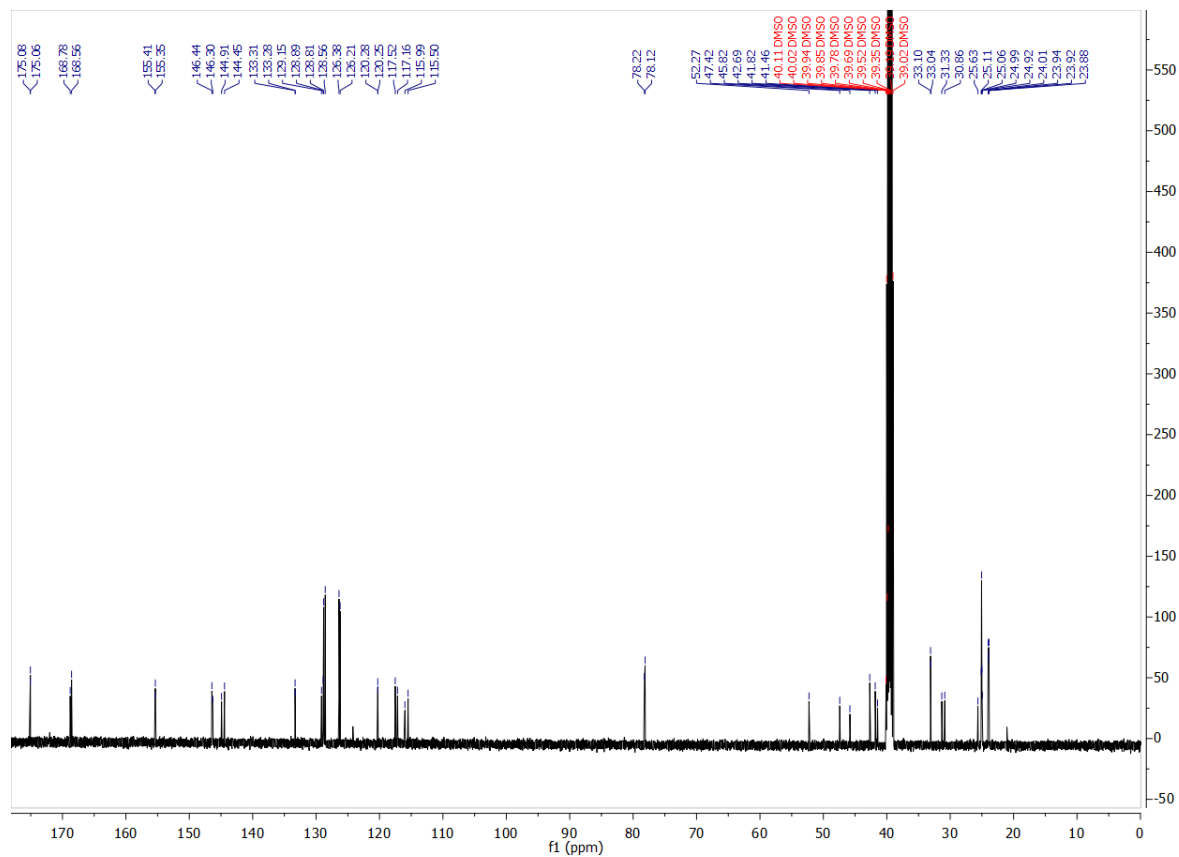
# COMPOUND INFORMATION

## Identity

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



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



# COMPOUND INFORMATION

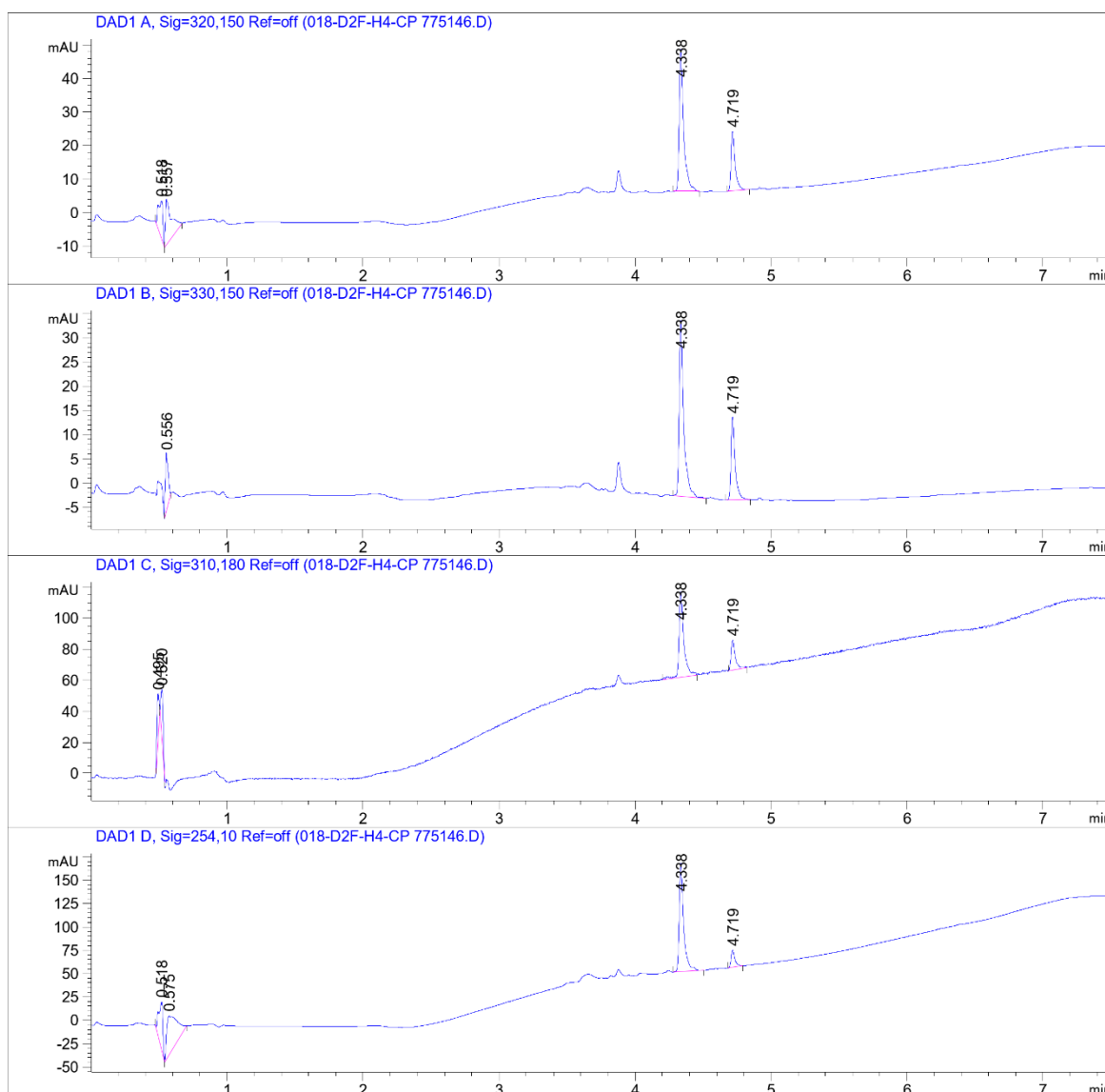
## Purity

Data File W:\analyti...\N\CGC\_ECH01-3\_SecondPass 2021-03-25 18-09-21\018-D2F-H4-CP 775146.D

Sample Name: CP 775146

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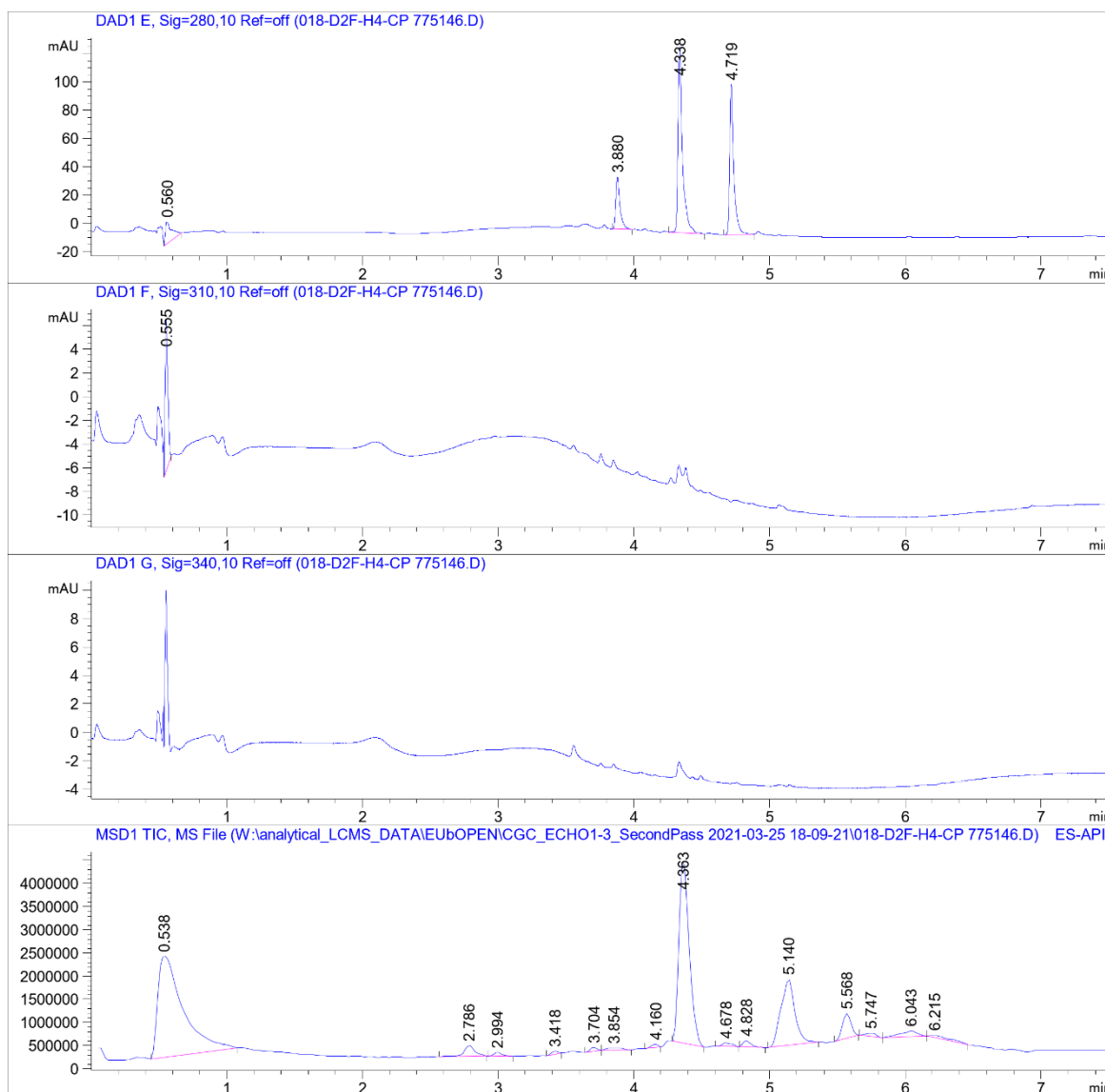
Acq. Operator	: SYSTEM	Seq. Line	: 18
Sample Operator	: SYSTEM		
Acq. Instrument	: LCMS test	Location	: D2F-H4
Injection Date	: 3/25/2021 9:19:43 PM	Inj	: 1
		Inj Volume	: Inj prog
Sequence File	: W:\analytical_LCMS_DATA\EUBOPEN\CGC_ECH01-3_SecondPass 2021-03-25 18-09-21 \CGC_ECH01-3_SecondPass.S		
Method	: 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...\N\CGC\_ECH01-3\_SecondPass 2021-03-25 18-09-21\018-D2F-H4-CP 775146.D

Sample Name: CP 775146



# COMPOUND INFORMATION



Data File W:\analyti...\N\CGC\_ECH01-3\_SecondPass 2021-03-25 18-09-21\018-D2F-H4-CP 775146.D

Sample Name: CP 775146

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
0.518	25	0.538	28108878	157.00 I
0.557	40	-	-	-
-	-	2.786	1241209	217.10 I
-	-	2.994	292907	274.30 I
-	-	3.418	212291	326.40 I
-	-	3.704	296369	214.10 I
-	-	3.854	412384	316.30 I 298.30 I 282.30 I 225.10 I 111.00 I
-	-	4.160	219673	280.20 I
4.338	97	4.363	21073622	424.30 I
4.719	37	4.678	356022	254.20 I
-	-	4.828	517532	280.20 I
-	-	5.140	10159769	282.30 I
-	-	5.568	2274933	381.30 I 359.30 I 341.30 I 284.30 I 282.30 I
-	-	5.747	369979	400.40 I 282.30 I
-	-	6.043	1025184	282.30 I
-	-	6.215	546708	282.30 I

