

COMPOUND INFORMATION

DG-172

CAS Registry No.: 1361504-77-9

Formal Name: (Z)-2-(2-bromophenyl)-3-(4-(4-methylpiperazin-1-yl)phenyl)acrylonitrile dihydrochloride

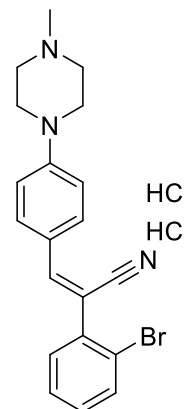
EUBOPEN ID: EUB0001483aCl

Molecular Formula: C₂₀H₂₂BrCl₂N₃

Molecular Weight: 455.22 g/mol

Smiles: CN1CCN(CC1)C2=CC=C(C=C2)C=C(C#N)C3=CC=CC=C3Br

Recommended concentration: 10 μM

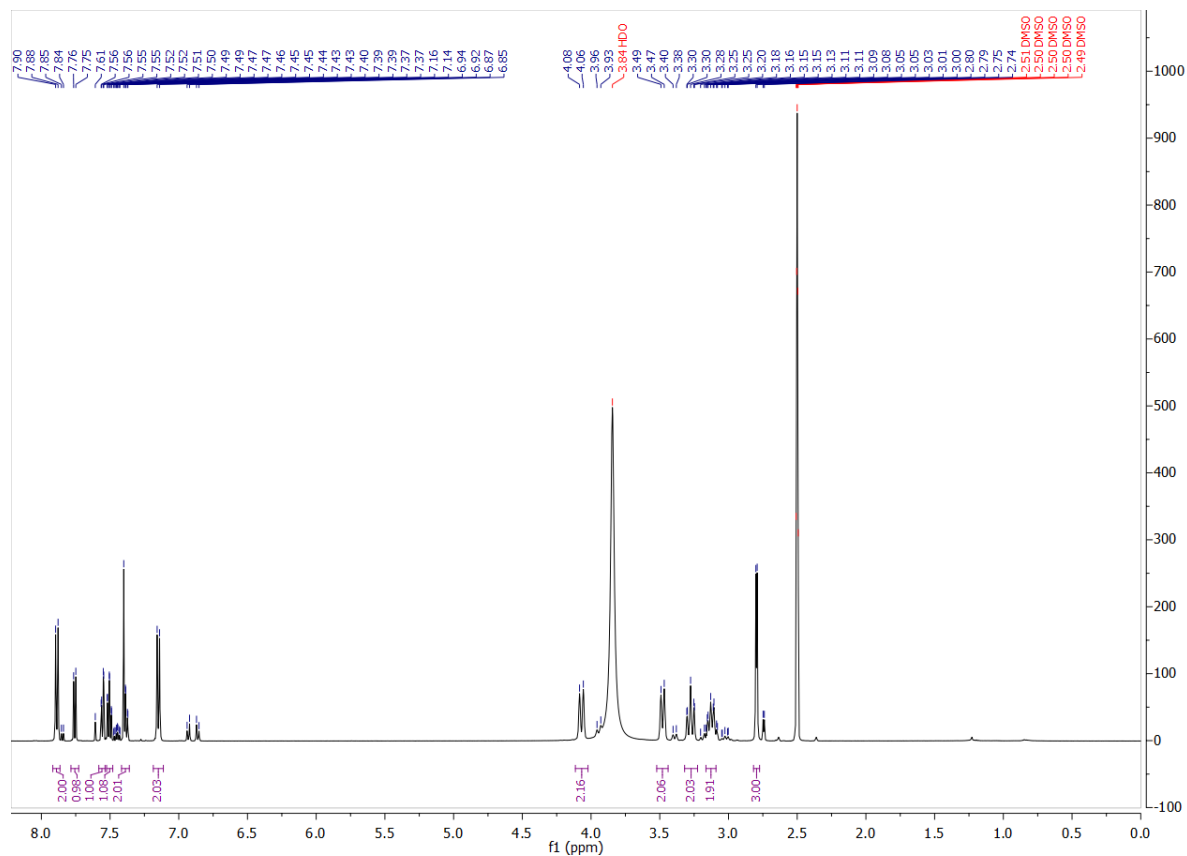


Biological activity

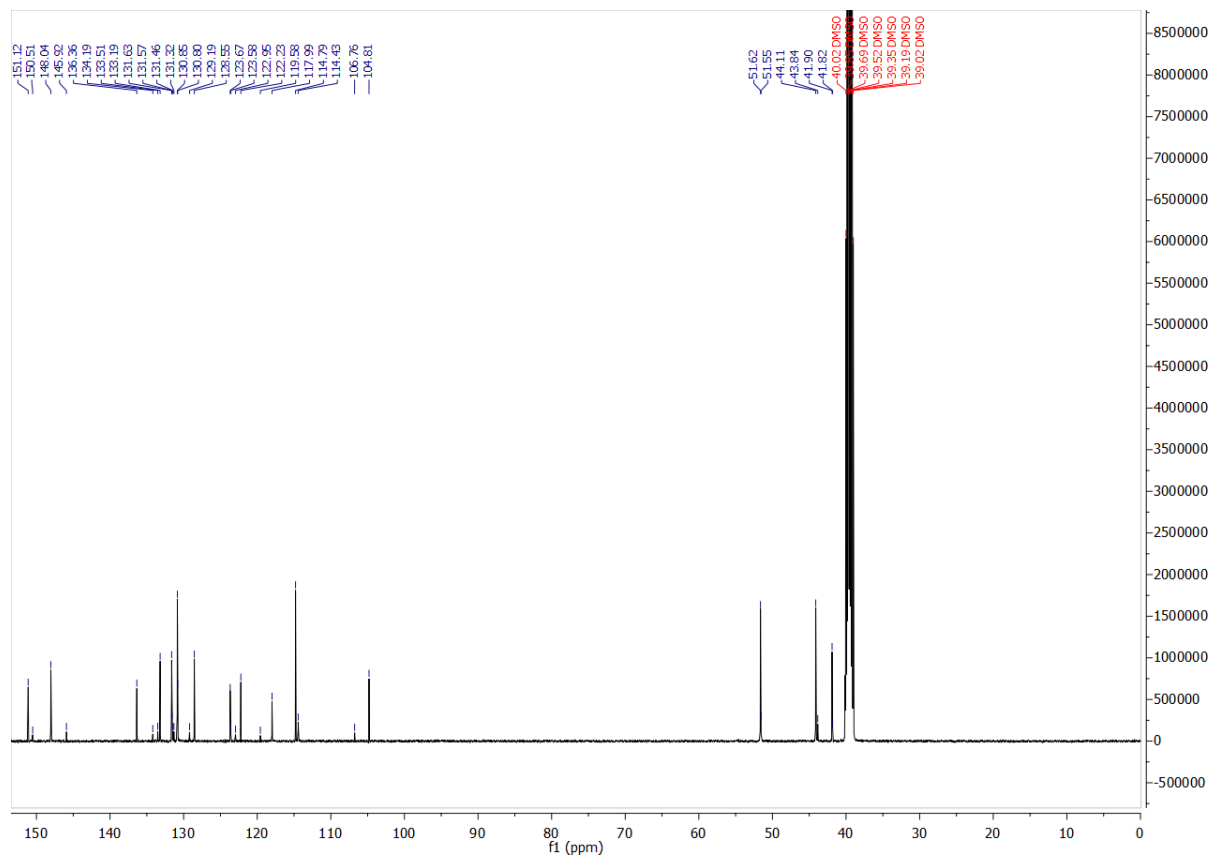
		Type	IC ₅₀ /EC ₅₀ [μM]	Reference
Main NR target:	NR1C2 (PPARδ)	Antagonist	1.8	inhouse
NR off-target:				

Identity

¹H NMR



¹³C NMR



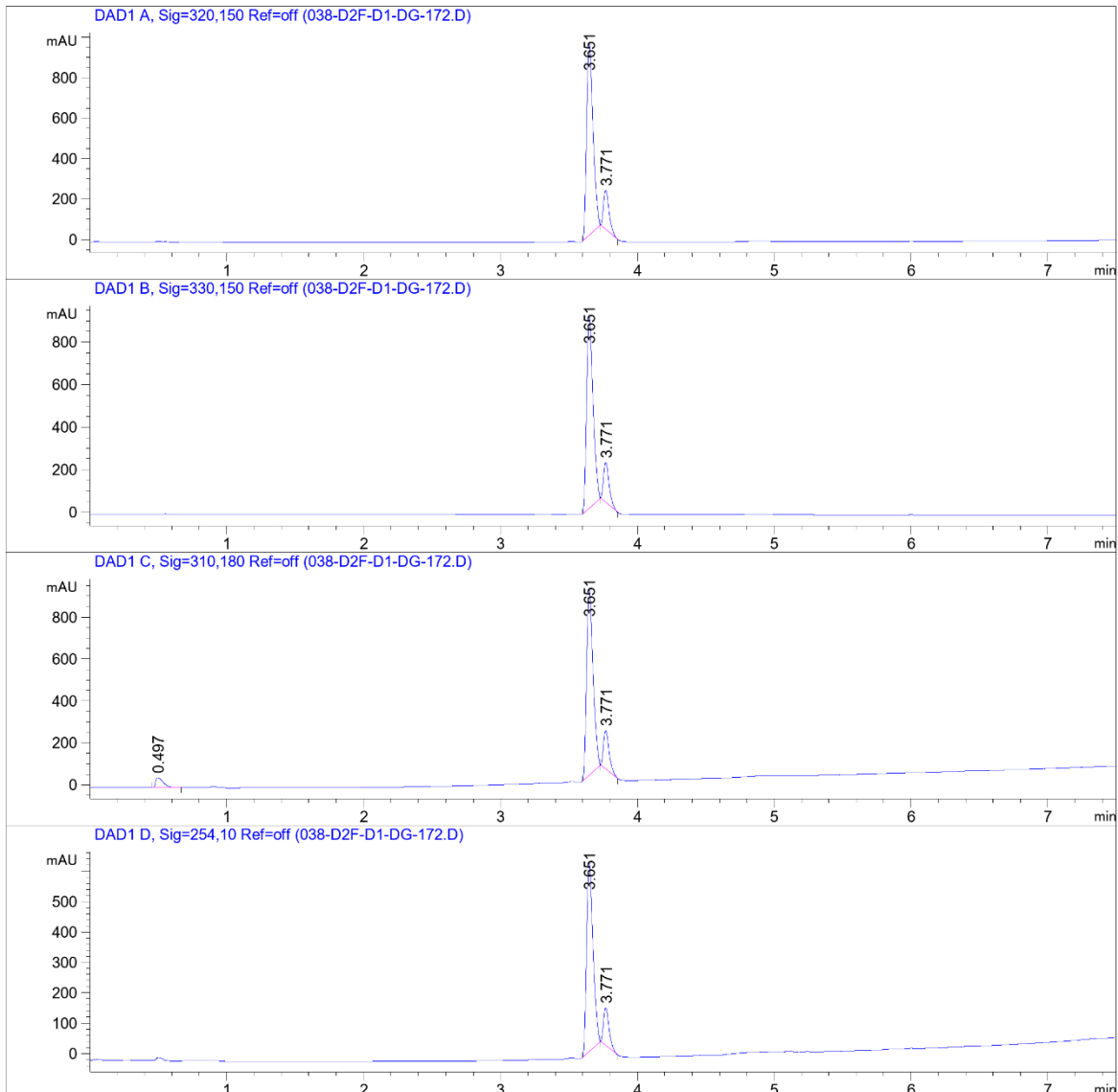
COMPOUND INFORMATION

Purity

Data File W:\analyti...bOPEN\CGC_wave3_2_FirstPass 2023-01-05 22-10-41\038-D2F-D1-DG-172.D

Sample Name: DG-172

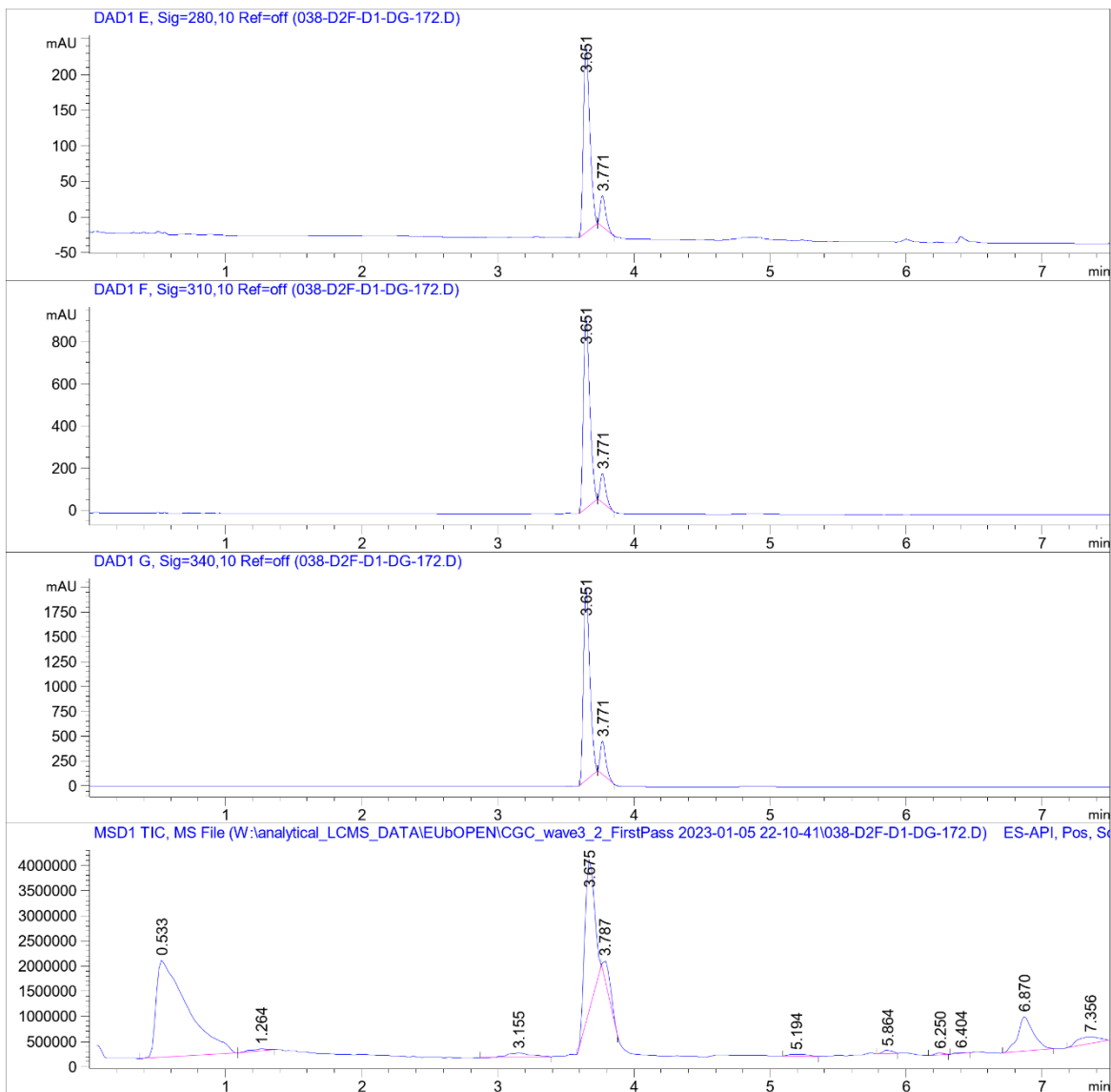
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=====
Acq. Operator   : SYSTEM                      Seq. Line :   38
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2F-D1
Injection Date  : 1/6/2023 5:02:53 AM         Inj       :    1
                                           Inj Volume: Inj prog
Sequence File   : W:\analytical_LCMS_DATA\EUBOPEN\CGC_wave3_2_FirstPass 2023-01-05 22-10-41
                  \CGC_wave3_2_FirstPass.S
Method          : W:\analytical_LCMS_DATA\EUBOPEN\CGC_wave3_2_FirstPass 2023-01-05 22-10-41
                  \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
=====
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Data File W:\analyti...bOPEN\CGC_wave3_2_FirstPass 2023-01-05 22-10-41\038-D2F-D1-DG-172.D

Sample Name: DG-172



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Data File W:\analyti...bOPEN\CGC_wave3_2_FirstPass 2023-01-05 22-10-41\038-D2F-D1-DG-172.D

Sample Name: DG-172

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

Spectra from peak tops.

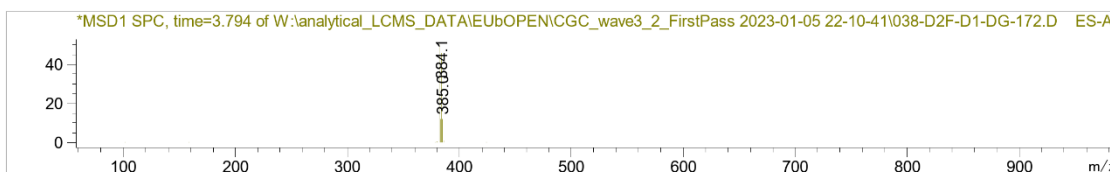
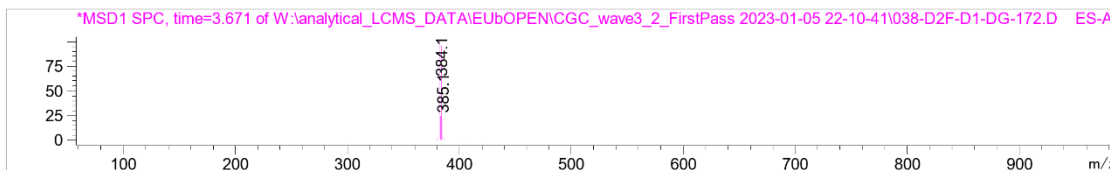
Noise Cutoff: 1000 counts.

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
-	-	0.533	30619936	157.10 I
-	-	1.264	319703	157.00 I
-	-	3.155	1029673	188.10 I 170.10 I
3.651	3092	3.675	14391690	384.10 I 382.10 I
3.771	552	3.787	1586792	384.10 I 382.00 I
-	-	5.194	344387	338.20 I 336.20 I 316.30 I 298.20 I 137.10 I
-	-	5.864	281108	318.20 I 296.20 I
-	-	6.250	171081	228.20 I 137.10 I
-	-	6.404	129809	282.20 I 254.20 I 137.10 I
-	-	6.870	5441228	282.20 I
-	-	7.356	1543379	400.30 I 282.20 I



COMPOUND INFORMATION

Biological activity

DG-172
PPAR δ - IC₅₀ 1.8 \pm 0.3 μ M
0.04 \pm 0.07 rem. activity

