

COMPOUND INFORMATION

LY2562175

CAS Registry No.: 1103500-20-4

Formal Name: 6-(4-((5-cyclopropyl-3-(2,6-dichlorophenyl)isoxazol-4-yl)methoxy)piperidin-1-yl)-1-methyl-1H-indole-3-carboxylic acid

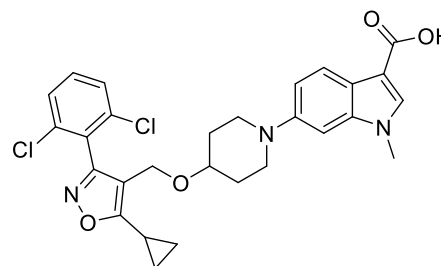
EUBOPEN ID: EUB0001173a

Molecular Formula: C₂₈H₂₇Cl₂N₃O₄

Molecular Weight: 540.44 g/mol

Smiles:
CN1C=C(C2=CC=C(C=C21)N3CC(C(C3)OCC4=C(ON=C4C5=C(C=CC=C5Cl)Cl)C6CC6)C(O)=O

Recommended concentration: 1 μM



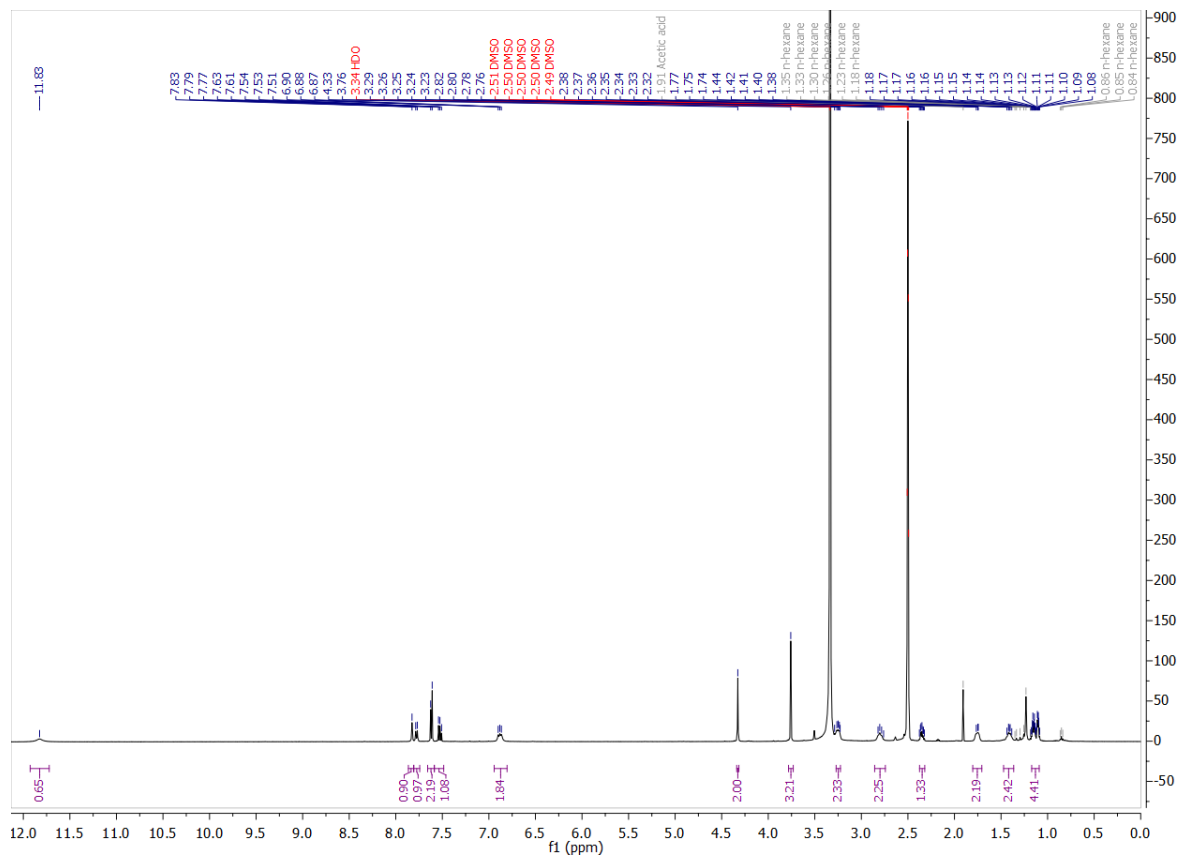
Biological activity

		Type	IC ₅₀ /EC ₅₀ [μM]	Reference
Main NR target:	NR1H4 (FXR)	Agonist	0.2	https://doi.org/10.1021/acs.jmedchem.5b01161
NR off-target:				

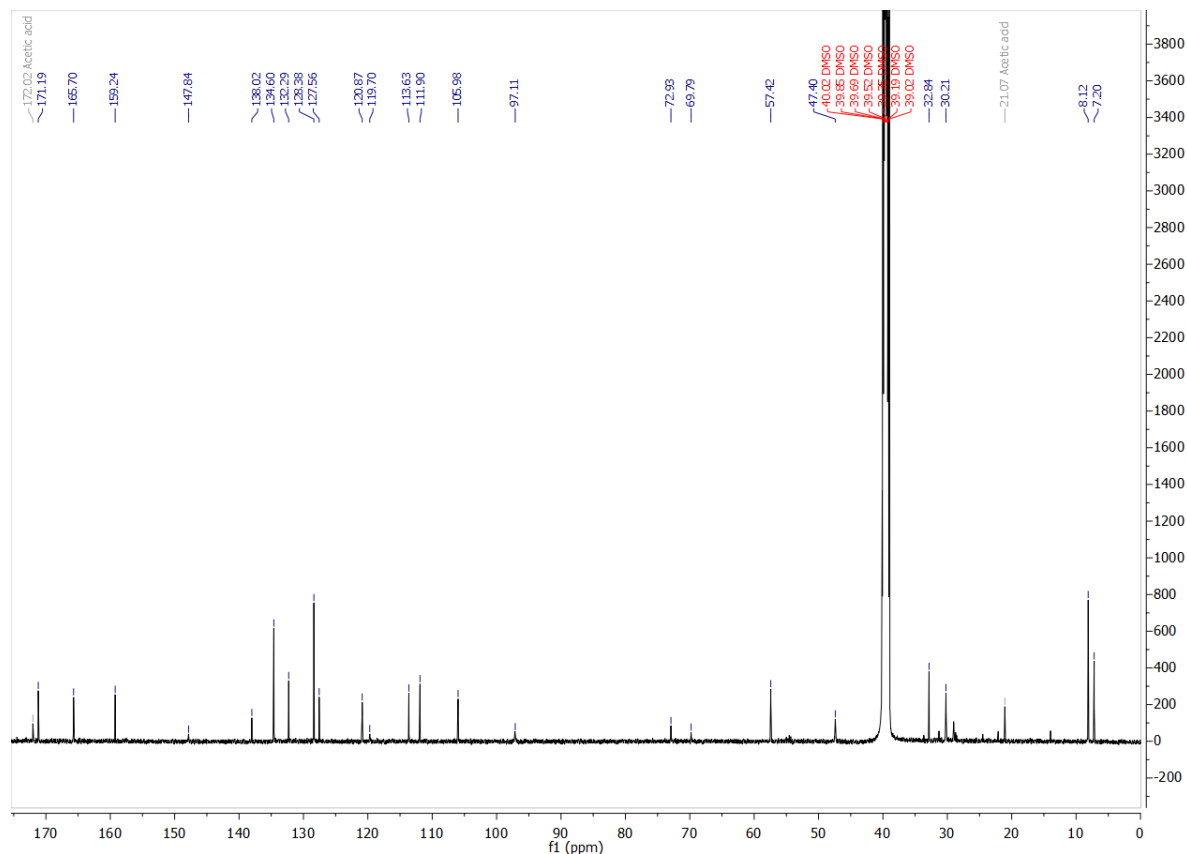
COMPOUND INFORMATION

Identity

¹H NMR



¹³C NMR



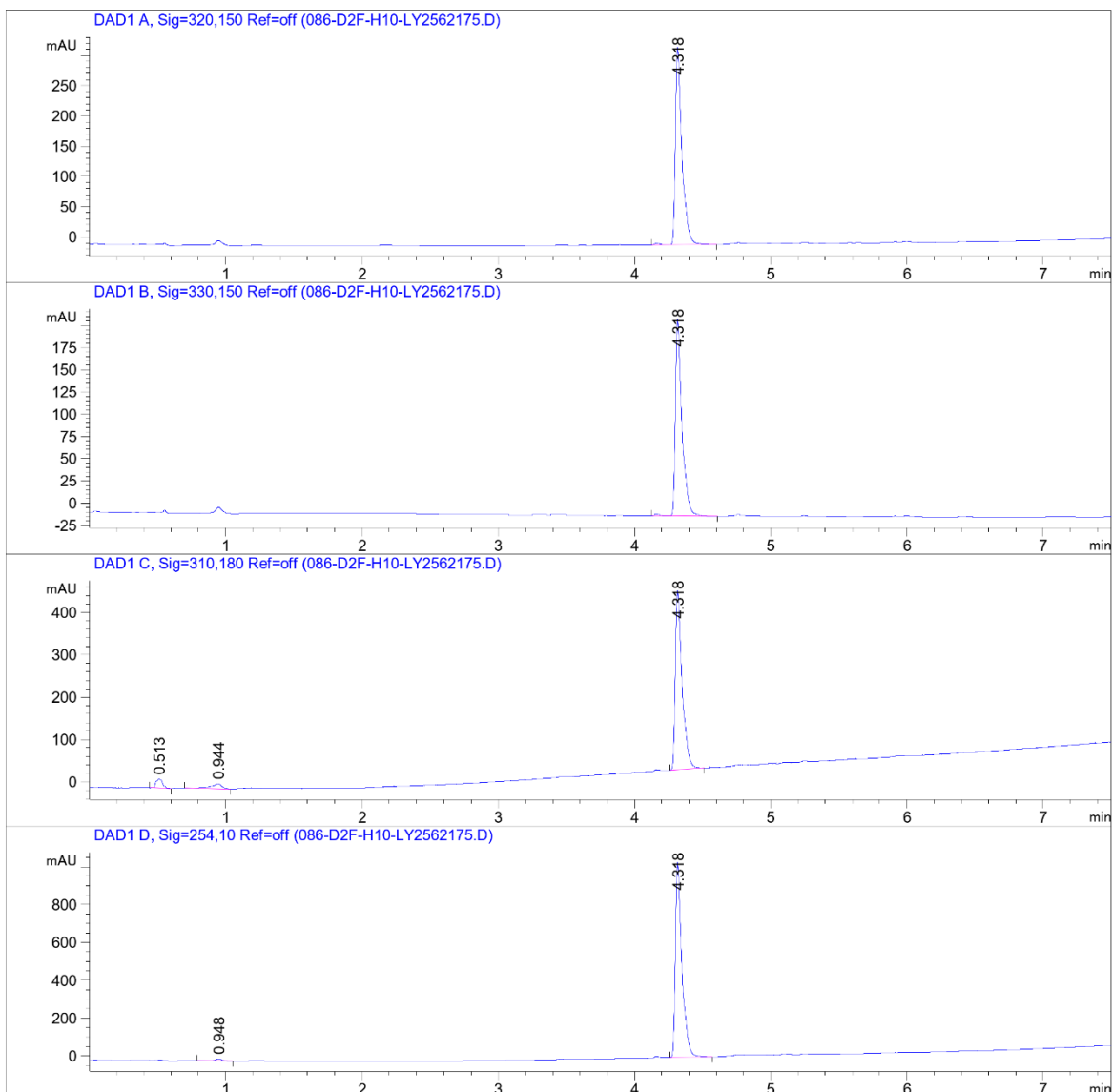
COMPOUND INFORMATION

Purity

Data File W:\analyti...\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\086-D2F-H10-LY2562175.D

Sample Name: LY2562175

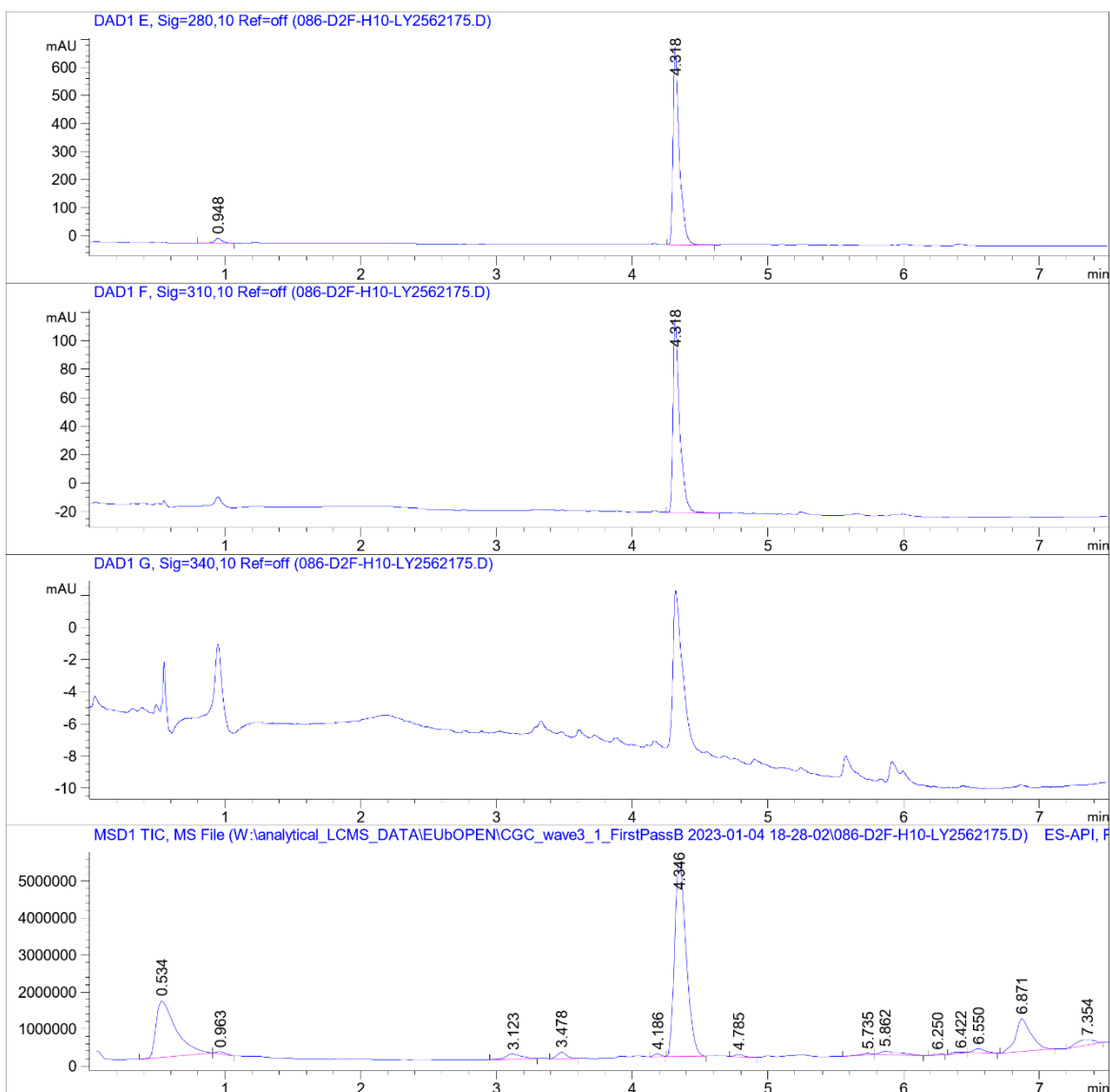
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=====
Acq. Operator   : SYSTEM                      Seq. Line :   86
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2F-H10
Injection Date  : 1/5/2023 10:10:47 AM       Inj       :    1
                                           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
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Data File W:\analyti...\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\086-D2F-H10-LY2562175.D

Sample Name: LY2562175



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Data File W:\analyti...\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\086-D2F-H10-LY2562175.D

Sample Name: LY2562175

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
-	-	0.534	15474488	157.00 I
-	-	0.963	282193	253.10 I 157.10 I
-	-	3.123	1123486	239.00 I 217.10 I 188.10 I
-	-	3.478	805334	369.10 I 367.00 I
-	-	4.186	265977	506.20 I
4.318	1077	4.346	31588666	542.10 I 540.10 I
-	-	4.785	285264	554.10 I 510.30 I 279.10 I 250.10 I 170.80 I 137.10 I
-	-	5.735	159735	280.20 I
-	-	5.862	867011	318.20 I 296.20 I
-	-	6.250	141678	228.20 I 137.10 I
-	-	6.422	182619	350.20 I 282.20 I 254.20 I 137.10 I
-	-	6.550	716134	507.30 I 485.20 I 280.20 I
-	-	6.871	7088273	282.20 I
-	-	7.354	1310393	400.30 I 282.20 I

