

CITCO

CAS Registry No.: 338404-52-7

Formal Name: (E)-6-(4-chlorophenyl)imidazo[2,1-b]thiazole-5-carbaldehyde O-(3,4-dichlorobenzyl) oxime

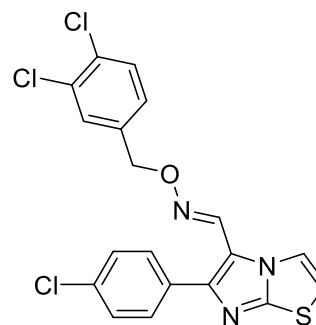
EUbOPEN ID EUB0001477a

Molecular Formula: C₁₉H₁₂Cl₃N₃OS

Molecular Weight: 436.74 g/mol

Smiles: ClC1=CC=C(C=C1)C2=C(N3C(SC=C3)=N2)/C=N/OCC4=CC(Cl)=C(C=C4)Cl

Recommended concentration: 1 μM

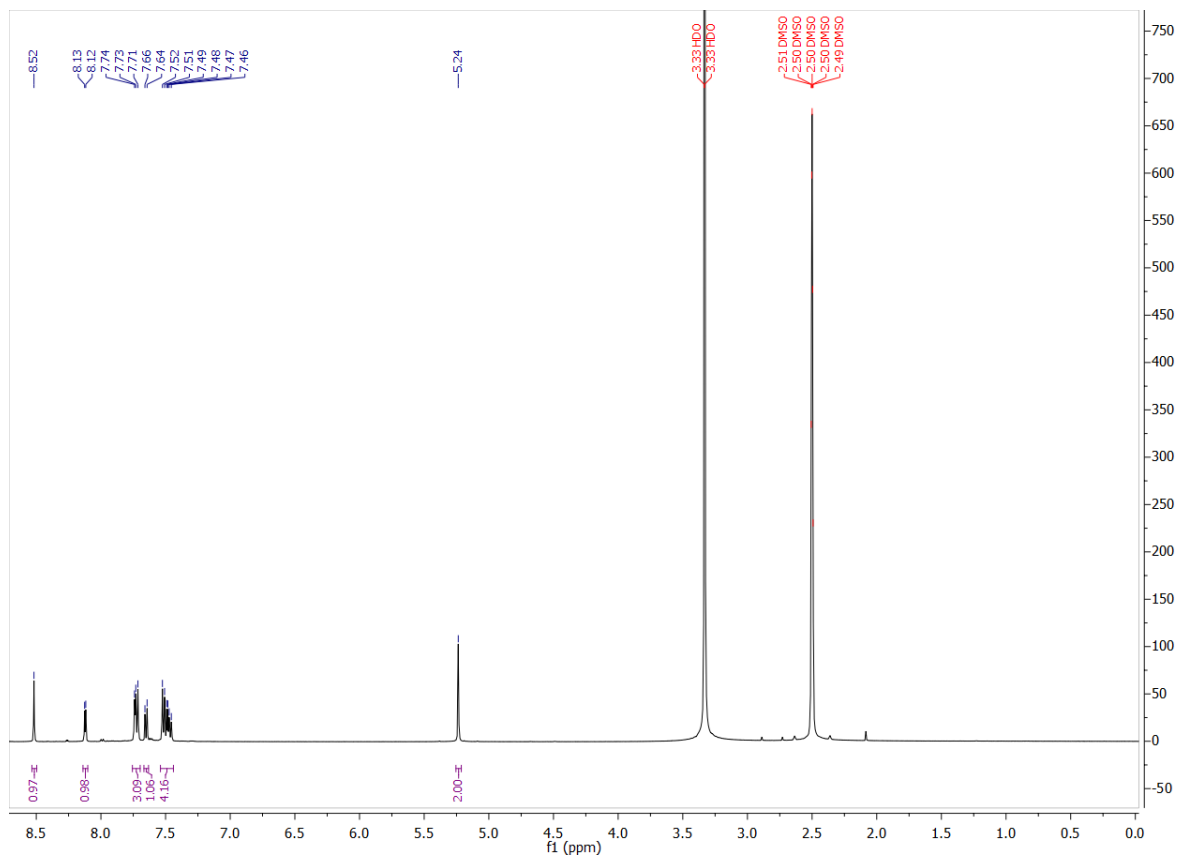


Biological activity

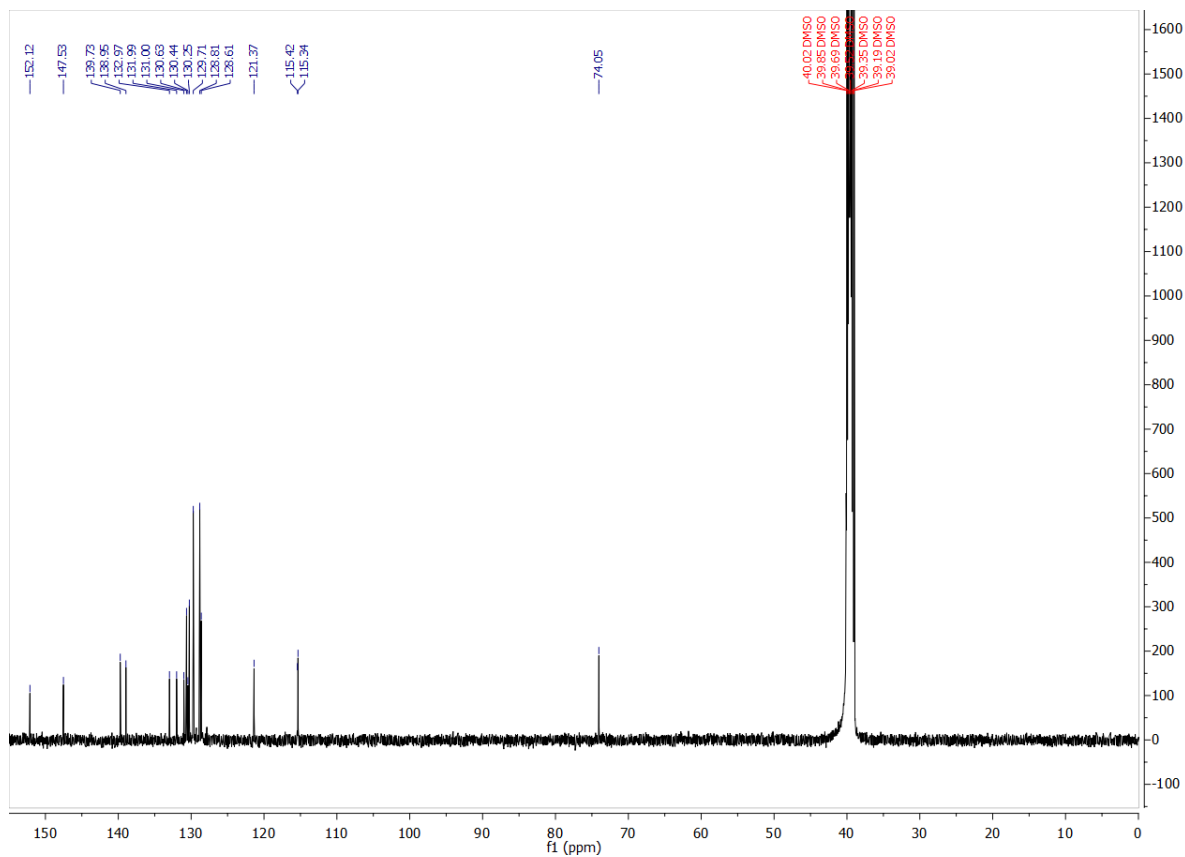
		Type	IC ₅₀ /EC ₅₀ [μM]	Reference
Main NR target:	NR1I3 (CAR)	Agonist	0.03	https://doi.org/10.1074/jbc.M300138200
NR off-targets:				

Identity

¹H NMR



¹³C NMR



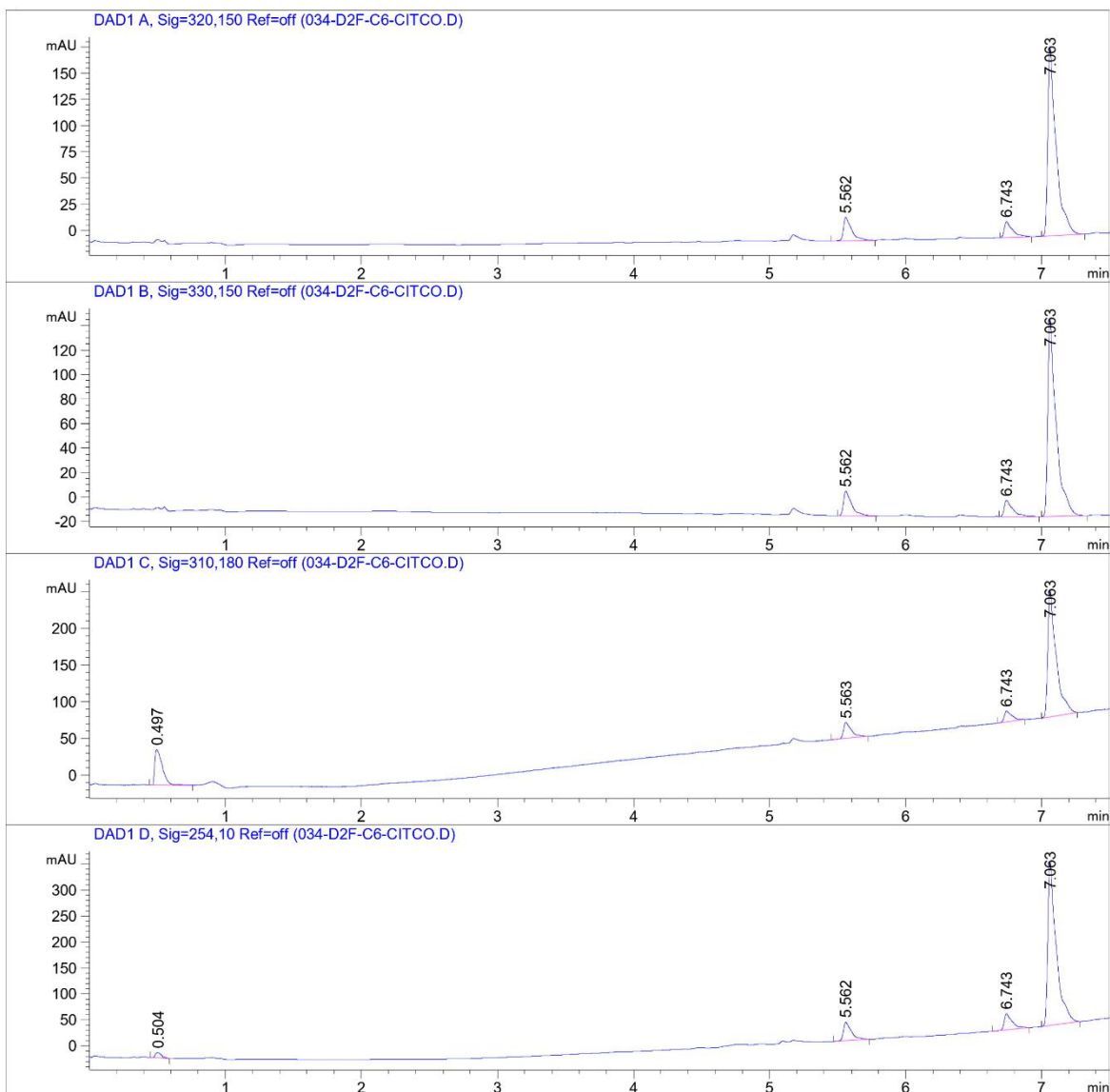
COMPOUND INFORMATION

Purity

Data File W:\analyti...UbOPEN\CGC_wave3_2_FirstPass 2023-01-05 22-10-41\034-D2F-C6-CITCO.D

Sample Name: CITCO

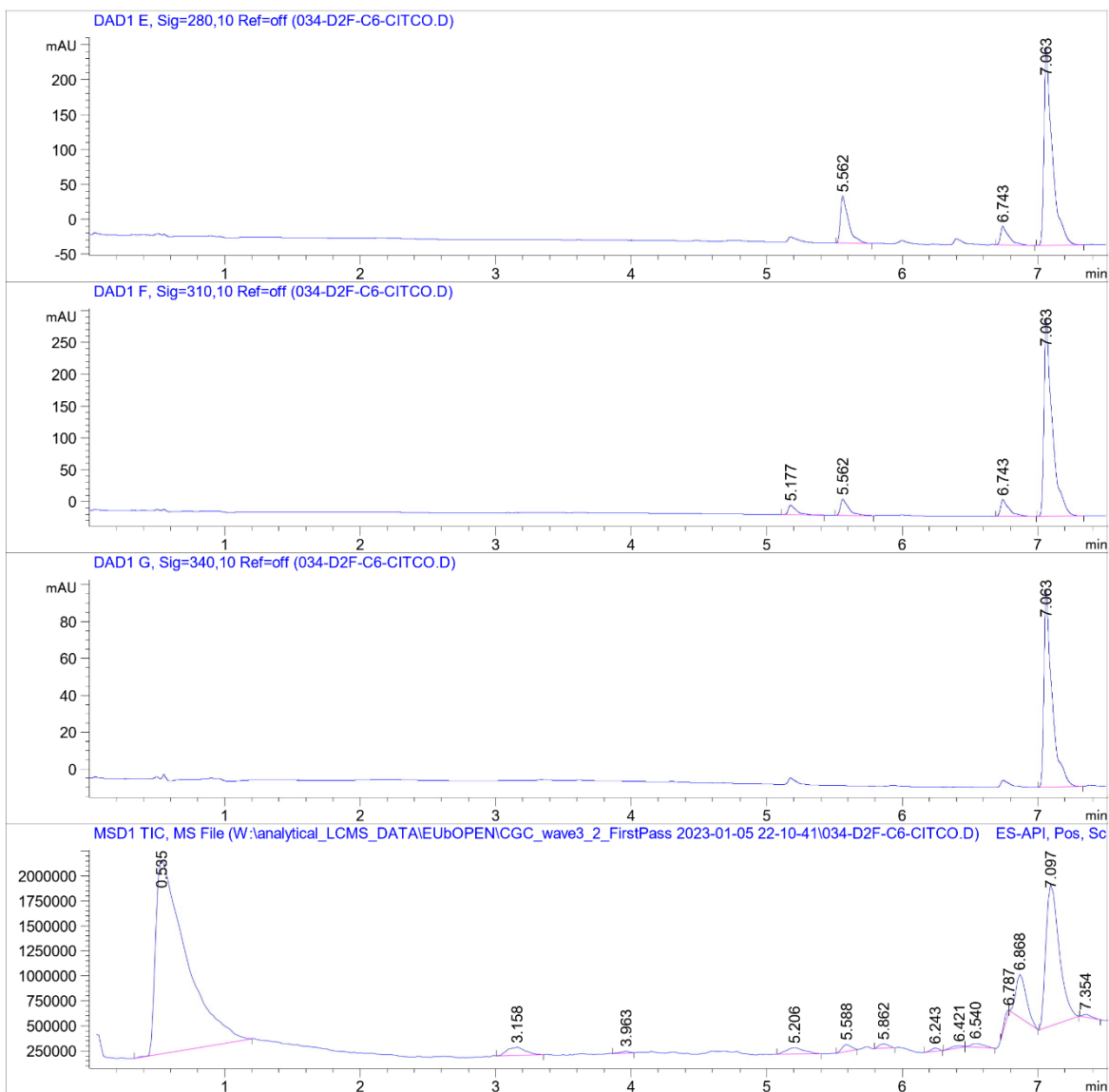
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=====
Acq. Operator   : SYSTEM                      Seq. Line :   34
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2F-C6
Injection Date  : 1/6/2023 4:18:40 AM         Inj       :    1
                                           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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COMPOUND INFORMATION

Data File W:\analyti...UbOPEN\CGC_wave3_2_FirstPass 2023-01-05 22-10-41\034-D2F-C6-CITCO.D

Sample Name: CITCO



COMPOUND INFORMATION

Data File W:\analyti...UbOPEN\CGC_wave3_2_FirstPass 2023-01-05 22-10-41\034-D2F-C6-CITCO.D

Sample Name: CITCO

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
-	-	0.535	30099000	157.00 I
-	-	3.158	785364	188.10 I 170.10 I
-	-	3.963	93181	420.10 I 216.10 I 210.60 I
-	-	5.206	603772	262.90 I
5.562	91	5.588	320900	260.00 I
-	-	5.862	207368	318.20 I 296.20 I
-	-	6.243	130524	228.20 I 137.10 I
-	-	6.421	135579	350.20 I 282.20 I 254.20 I 137.10 I
-	-	6.540	264372	280.20 I
6.743	63	6.787	164896	438.00 I 435.90 I 256.20 I
-	-	6.868	2328094	282.20 I
7.063	760	7.097	9609414	437.90 I 435.90 I
-	-	7.354	125122	400.30 I 282.20 I

