

Cintirorgon

CAS Registry No.: 2055536-64-4

Formal Name: (S)-3-(6-(3-(difluoromethoxy)-5-fluorophenyl)-4-((3-(trifluoromethyl)phenyl)sulfonyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-yl)-2,2-dimethylpropanoic acid

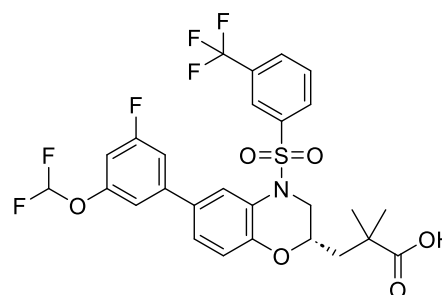
EUBOPEN ID: EUB0001172

Molecular Formula: C₂₇H₂₃F₆NO₆S

Molecular Weight: 603.53 g/mol

Smiles:
O=S(N1C2=C(O[C@H](C1)CC(C)(C(O)=O)C)C=CC(C3=CC(F)=CC(O)C(F)F)=C3)=C2)(C4=CC(C(F)F)F)=CC=C4)=O

Recommended concentration: 1 μM



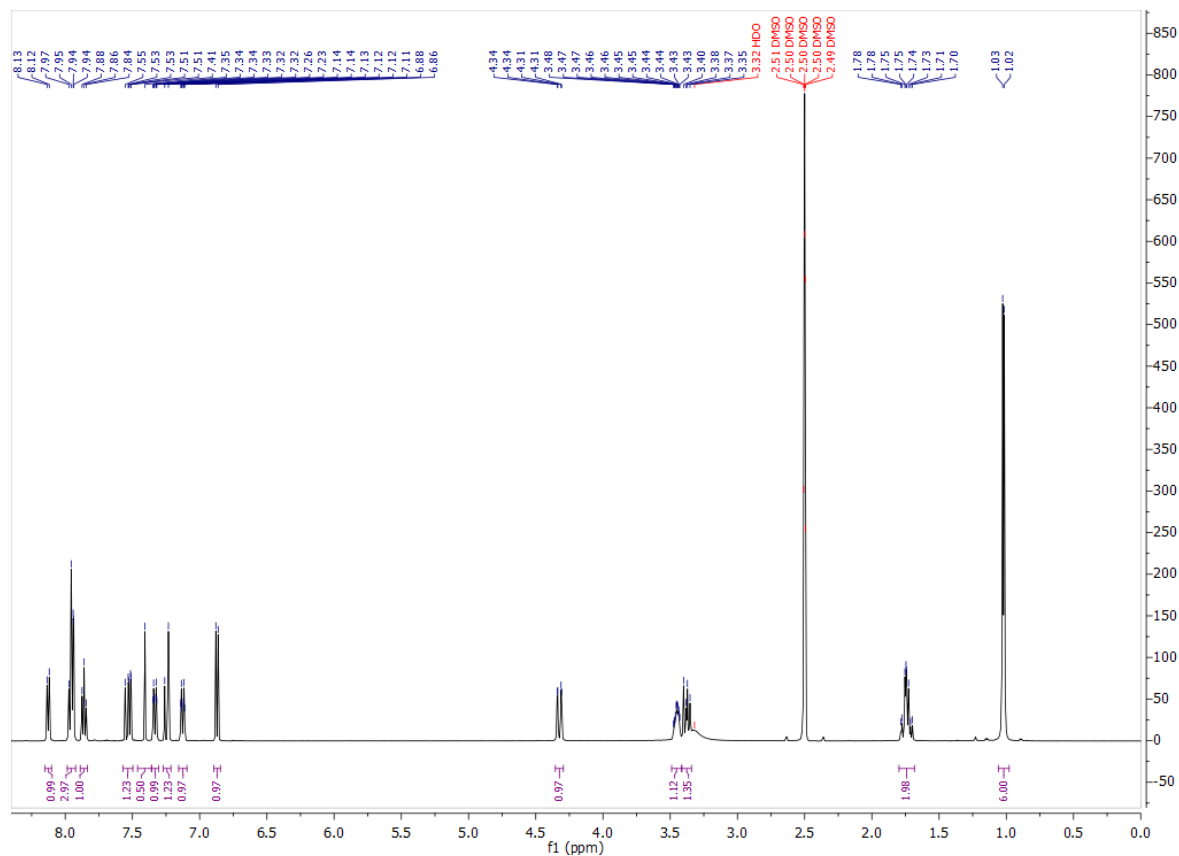
Biological activity

		Type	IC ₅₀ /EC ₅₀ [μM]	Reference
Main NR target:	NR1F3 (RORγ)	Agonist	0.021	inhouse
NR off-target:				

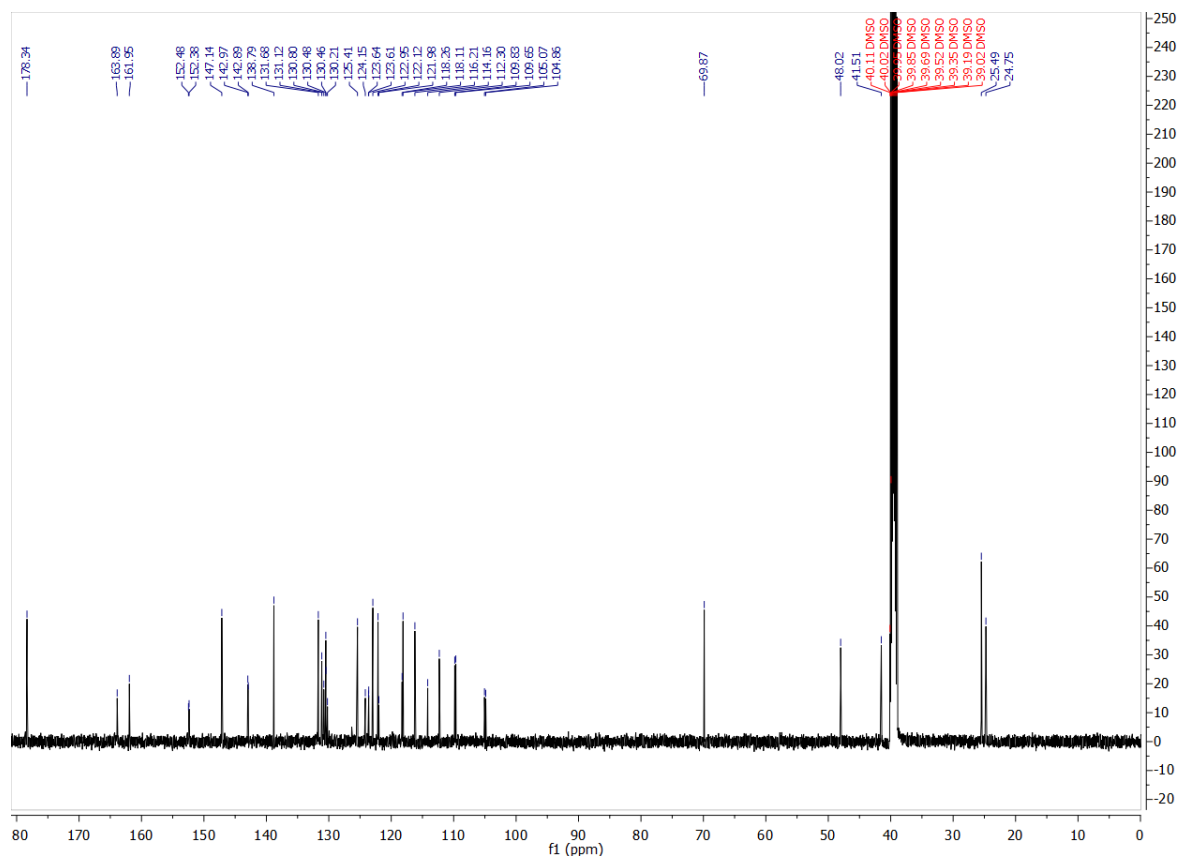
COMPOUND INFORMATION

Identity

¹H NMR



¹³C NMR



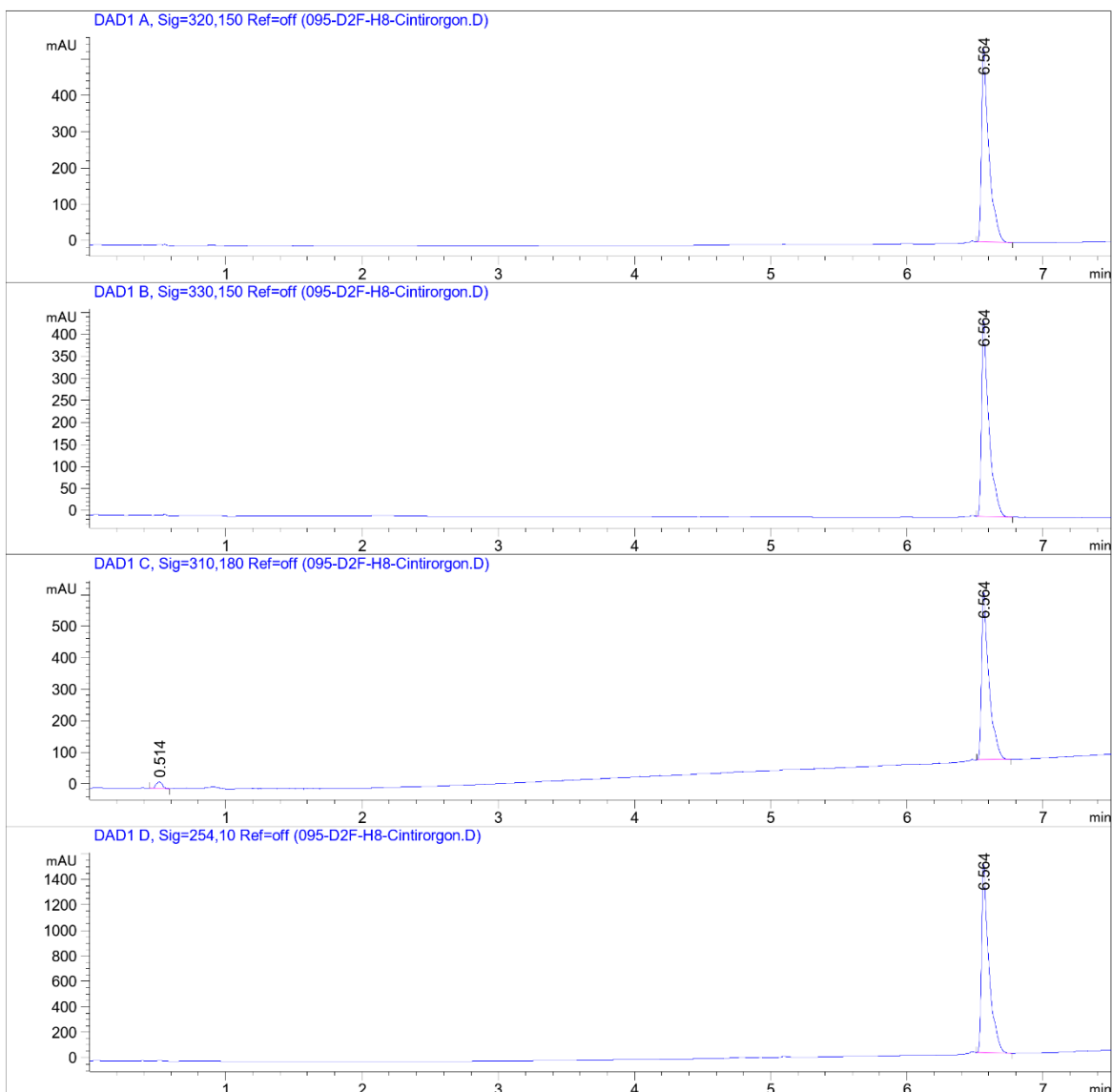
COMPOUND INFORMATION

Purity

Data File W:\analyti...CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\095-D2F-H8-Cintirorgon.D

Sample Name: Cintirorgon

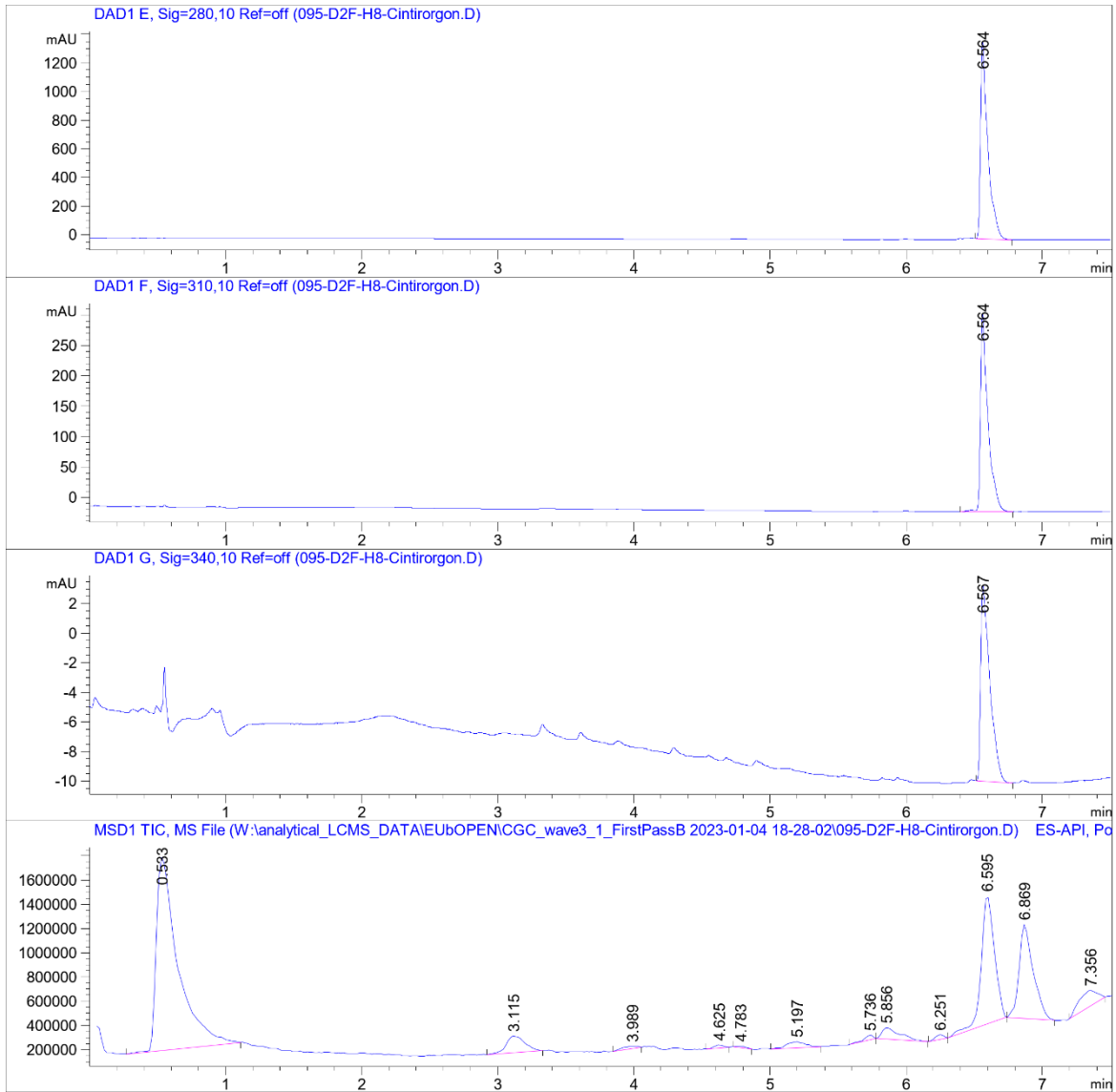
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=====
Acq. Operator   : SYSTEM                      Seq. Line :   95
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2F-H8
Injection Date  : 1/5/2023 11:50:22 AM       Inj       :    1
                                           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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COMPOUND INFORMATION

Data File W:\analyti...CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\095-D2F-H8-Cintirorgon.D

Sample Name: Cintirorgon



COMPOUND INFORMATION

Data File W:\analyti...CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\095-D2F-H8-Cintirorgon.D

Sample Name: Cintirorgon

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

Spectra from peak tops.

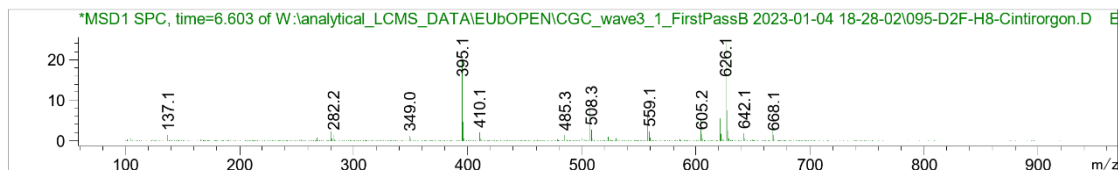
Noise Cutoff: 1000 counts.

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	17619570	157.00 I
-	-	3.115	1310425	239.10 I 217.00 I
-	-	3.989	162561	216.10 I 200.00 I 170.90 I 159.00 I 137.10 I
-	-	4.625	118658	170.80 I 158.10 I 137.10 I
-	-	4.783	74052	279.10 I 137.10 I
-	-	5.197	490456	510.40 I 338.20 I 336.20 I 316.20 I 298.20 I 252.10 I 137.10 I 105.10 I
-	-	5.736	167582	280.20 I
-	-	5.856	852424	318.20 I 296.20 I
-	-	6.251	176272	228.20 I 137.10 I
6.564	1980	6.595	7219776	626.10 I 395.10 I
-	-	6.869	5583937	282.20 I
-	-	7.356	1240152	400.30 I 282.20 I



COMPOUND INFORMATION

Biological activity

Cintirorgon
ROR γ - EC₅₀ 0.021 \pm 0.009 μ M
2.4 \pm 0.1 fold activation

