

Meclizine (dihydrochloride)

CAS Registry No.: 1104-22-9

Formal Name: 1-((4-chlorophenyl)(phenyl)methyl)-4-(3-methylbenzyl)piperazine dihydrochloride

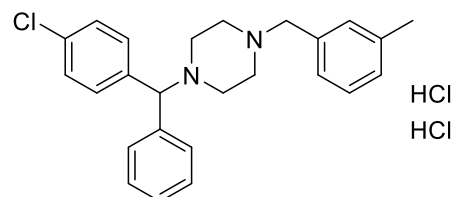
EUBOPEN ID EUB0000551aCl

Molecular Formula: C₂₅H₂₉Cl₃N₂

Molecular Weight: 462.14 g/mol

Smiles:
CC1=CC(CN2CCN(C(C3=CC=C(Cl)C=C3)C4=CC=CC=C4)CC2)=CC=C1.Cl.Cl

Recommended concentration: 1 μM



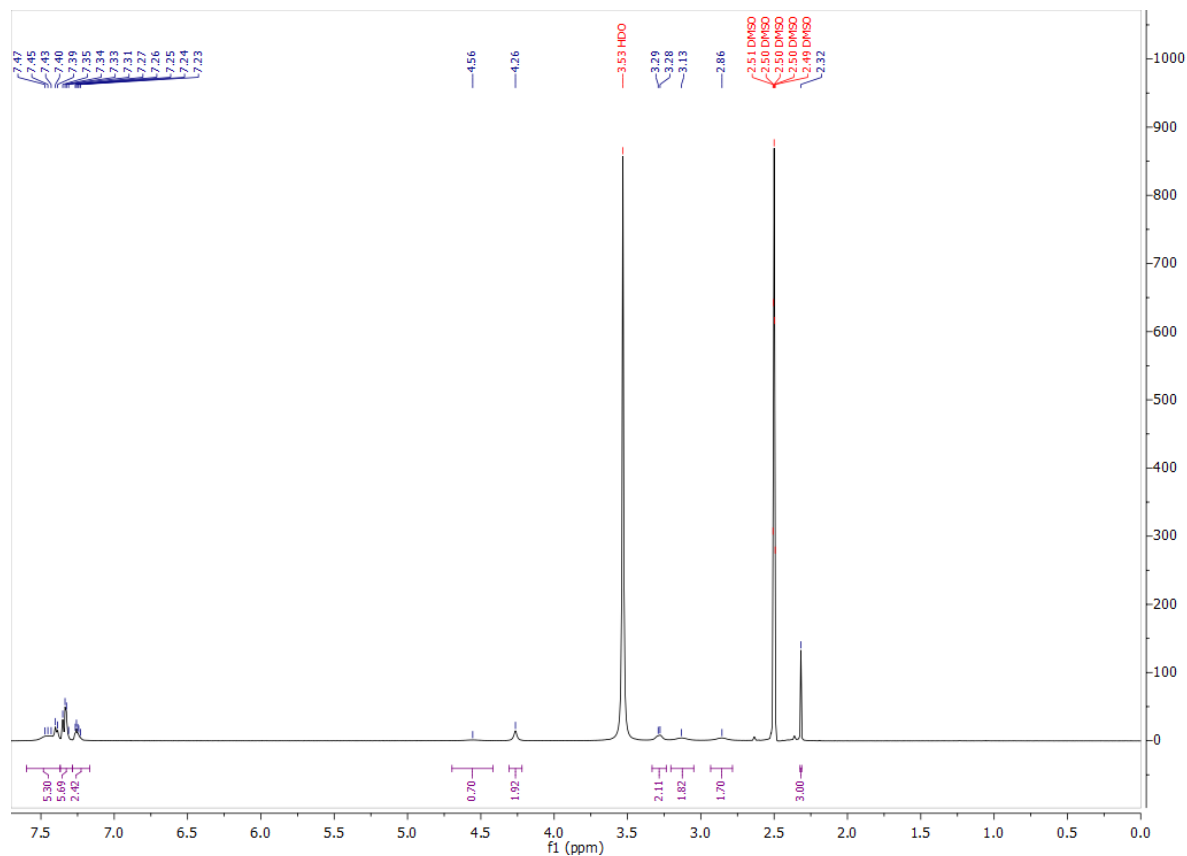
Biological activity

		Type	IC ₅₀ /EC ₅₀ [μM]	Reference
Main NR target:	NR113 (CAR)	inv. Agonist	0.06	https://doi.org/10.1210/me.2004-0046
NR off-target:				

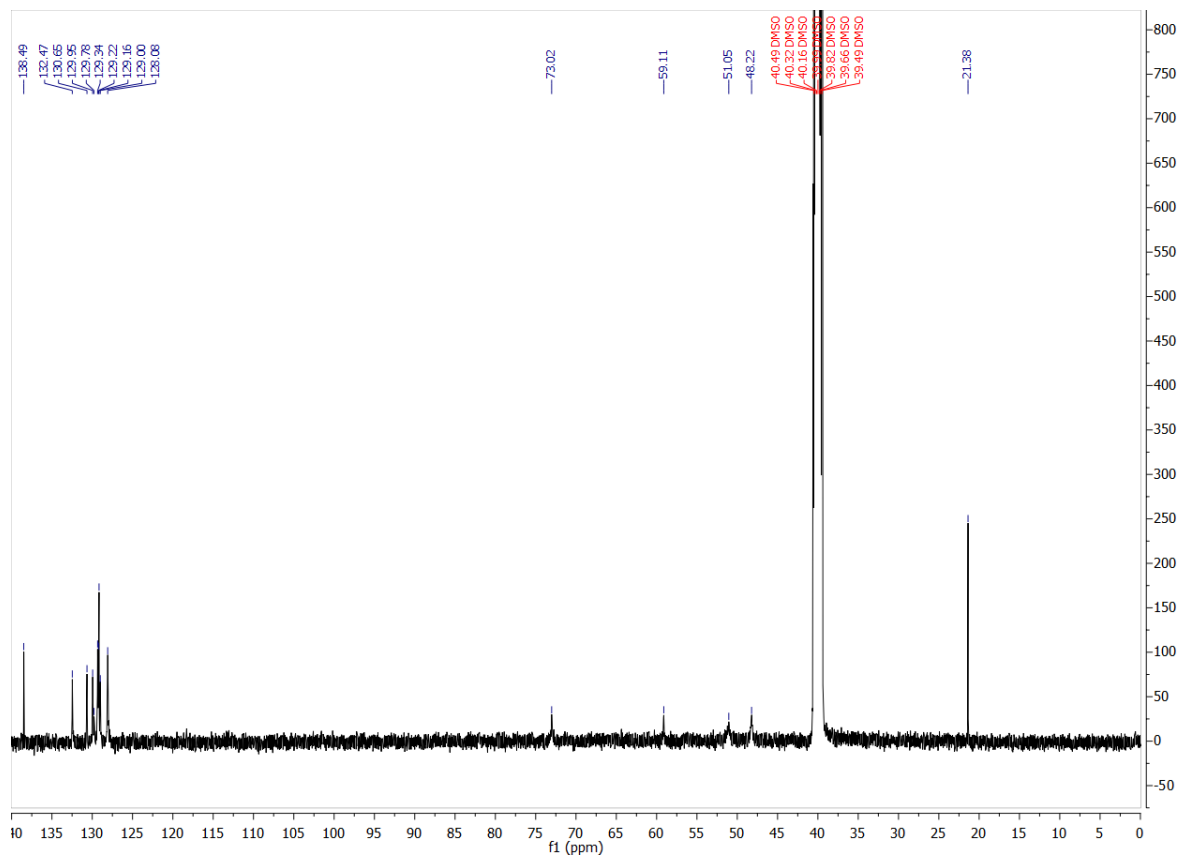
COMPOUND INFORMATION

Identity

¹H NMR



¹³C NMR



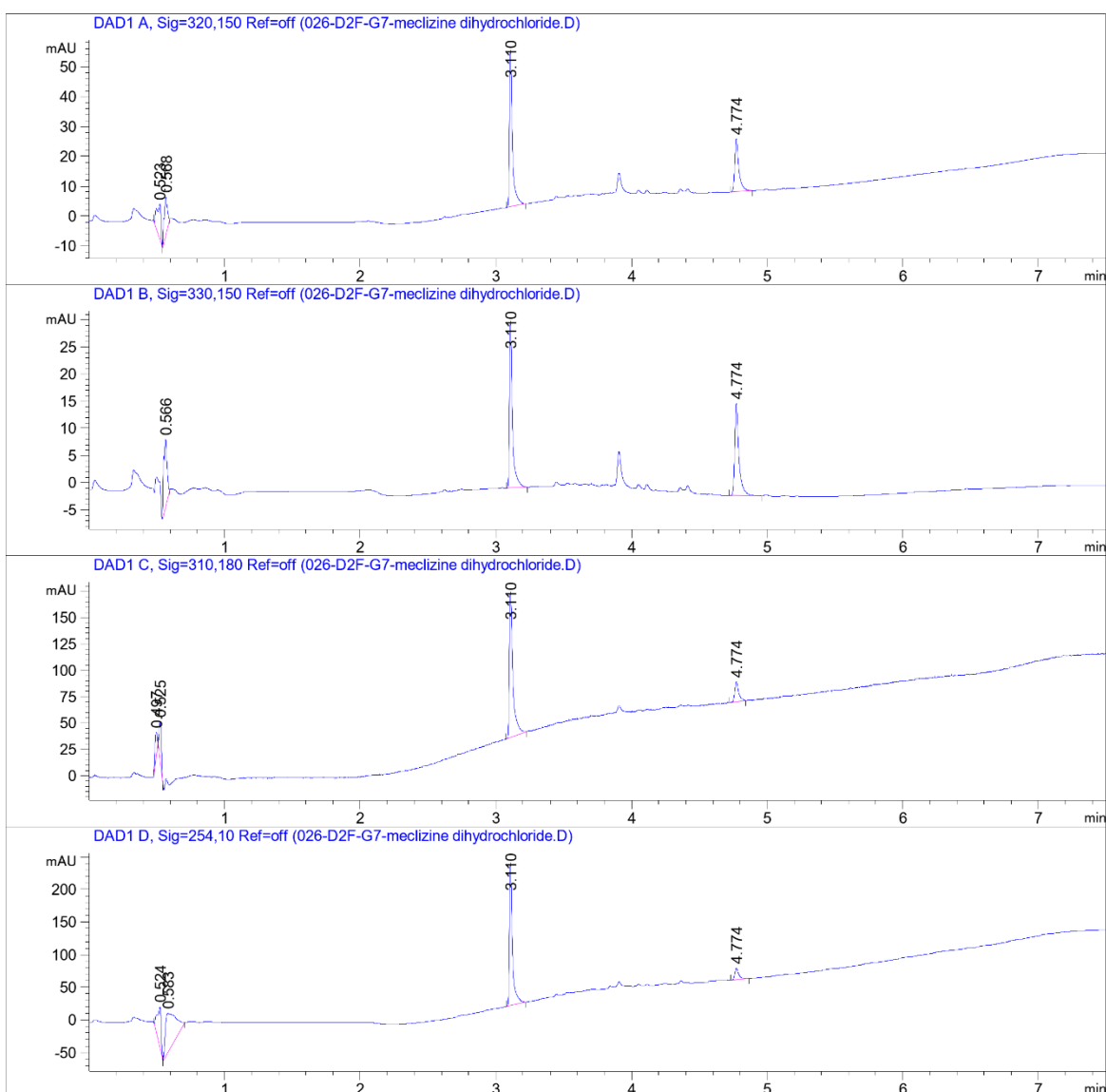
COMPOUND INFORMATION

Purity

Data File W:\analyti...condPass 2021-03-23 18-53-53\026-D2F-G7-meclizine dihydrochloride.D

Sample Name: meclizine dihydrochloride

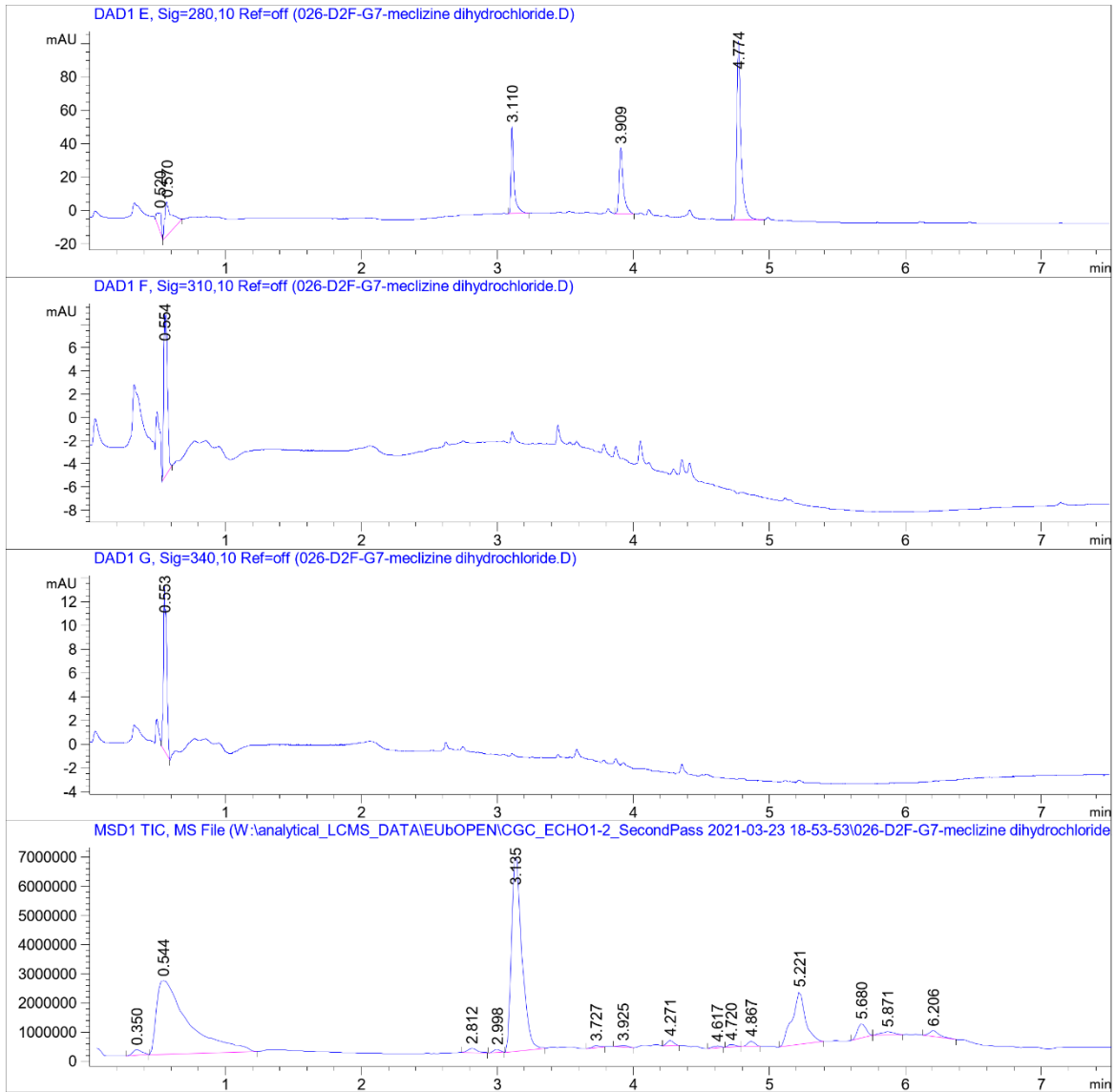
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=====
Acq. Operator   : SYSTEM                               Seq. Line :   26
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                           Location  : D2F-G7
Injection Date  : 3/23/2021 11:34:52 PM              Inj       :    1
                                                    Inj Volume: Inj prog
Sequence File   : W:\analytical_LCMS_DATA\EUBOPEN\CGC_ECH01-2_SecondPass 2021-03-23 18-53-53
                  \CGC_ECH01-2_SecondPass.S
Method          : W:\analytical_LCMS_DATA\EUBOPEN\CGC_ECH01-2_SecondPass 2021-03-23 18-53-53
                  \CGL_SECONDPASS_NONPOLCOMP_VIAL2+4_20210323.M (Sequence Method)
Last changed    : 3/23/2021 6:50:05 PM by SYSTEM
Method Info     : CGL wellplate, 0.5 uL of 10 mM DMSO. Dilution with MeCN only (9+9 uL)
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COMPOUND INFORMATION

Data File W:\analyti...condPass 2021-03-23 18-53-53\026-D2F-G7-meclizine dihydrochloride.D

Sample Name: meclizine dihydrochloride



COMPOUND INFORMATION



Data File W:\analyti...condPass 2021-03-23 18-53-53\026-D2F-G7-meclizine dihydrochloride.D

Sample Name: meclizine dihydrochloride

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
-	-	0.350	866279	200.00 I 183.00 I 159.00 I
0.523	24	0.544	41320044	157.10 I
0.568	21	-	-	-
-	-	2.812	693982	217.10 I
-	-	2.998	340473	274.20 I
3.110	79	3.135	35698364	391.20 I
-	-	3.727	276232	391.20 I 214.10 I
-	-	3.925	275017	512.50 I
-	-	4.271	645780	296.20 I
-	-	4.617	221542	228.20 I
4.774	37	4.720	291088	254.20 I
-	-	4.867	644958	280.30 I
-	-	5.221	12461739	282.30 I
-	-	5.680	2044310	359.30 I 284.30 I 282.30 I
-	-	5.871	762513	400.30 I 282.30 I
-	-	6.206	988690	338.30 I 282.20 I

