

COMPOUND INFORMATION

SR8278

CAS Registry No.: 1254944-66-5

Formal Name: Ethyl 2-(5-(methylthio)thiophene-2-carbonyl)-1,2,3,4-tetrahydroisoquinoline-3-carboxylate

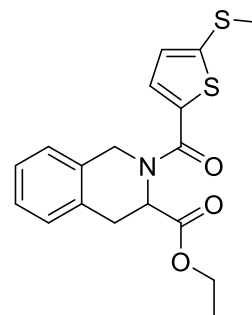
EUBOPEN ID: EUB0001153a

Molecular Formula: C₁₈H₁₉NO₃S₂

Molecular Weight: 361.47 g/mol

Smiles: CCOC(=O)C1CC2=CC=CC=C2CN1C(=O)C3=CC=C(S3)SC

Recommended concentration: 10 μM

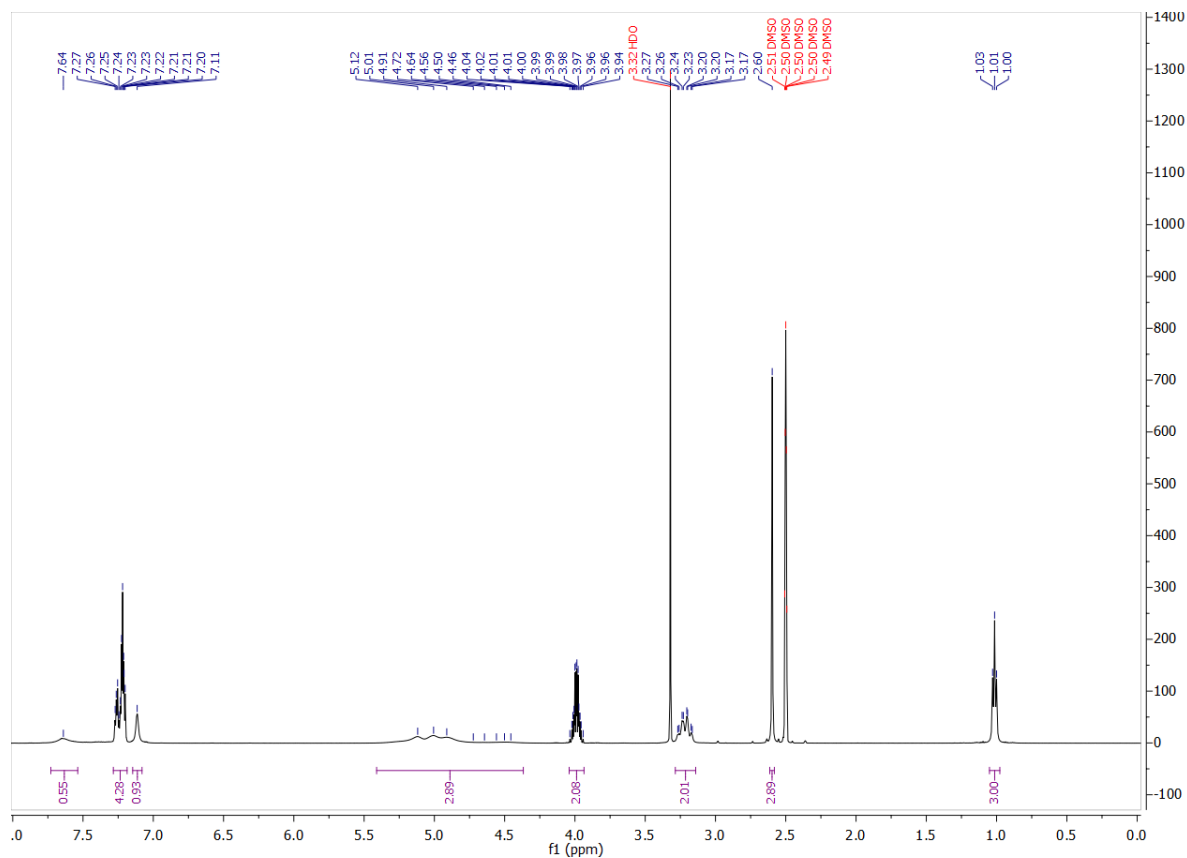


Biological activity

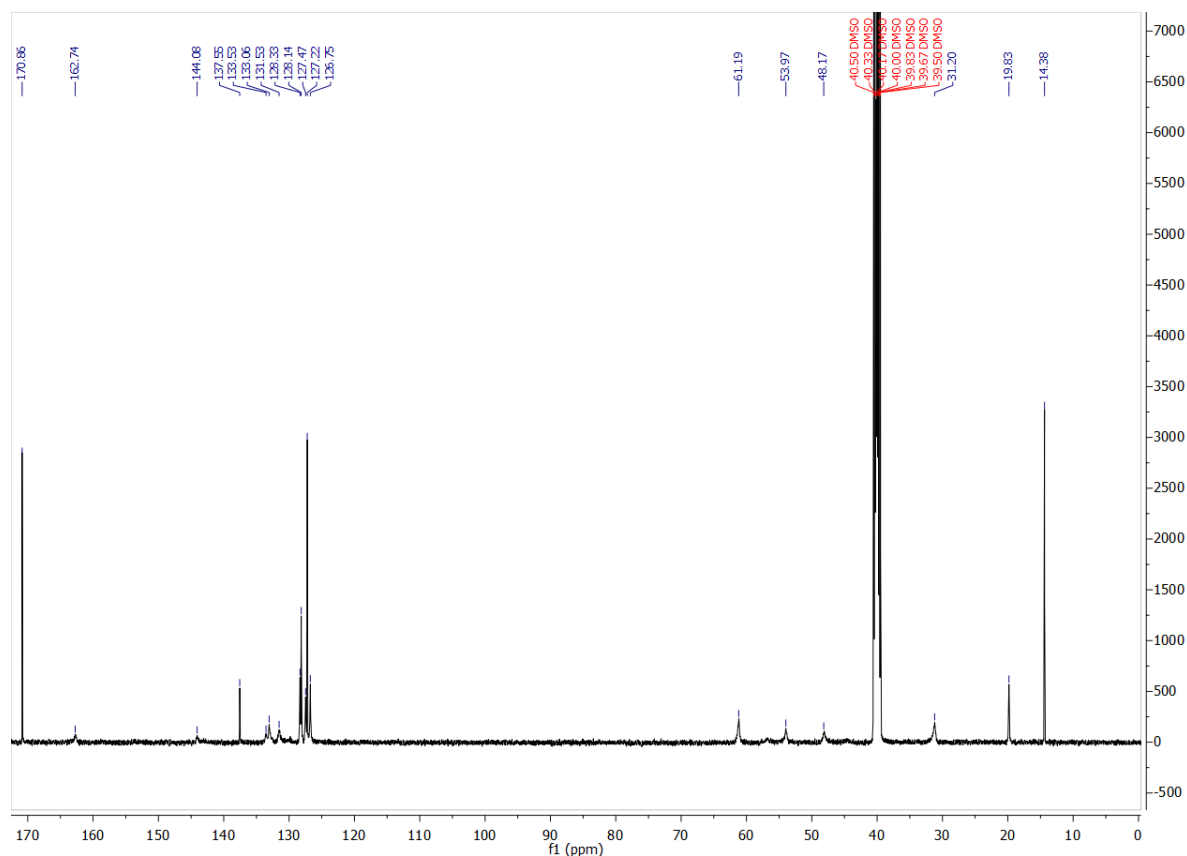
		Type	IC ₅₀ /EC ₅₀ [μM]	Reference
Main NR target:	NR1D1 (revERBα)	Antagonist	0.5	https://doi.org/10.1021/cb1002575
NR off-target:				

Identity

¹H NMR



¹³C NMR



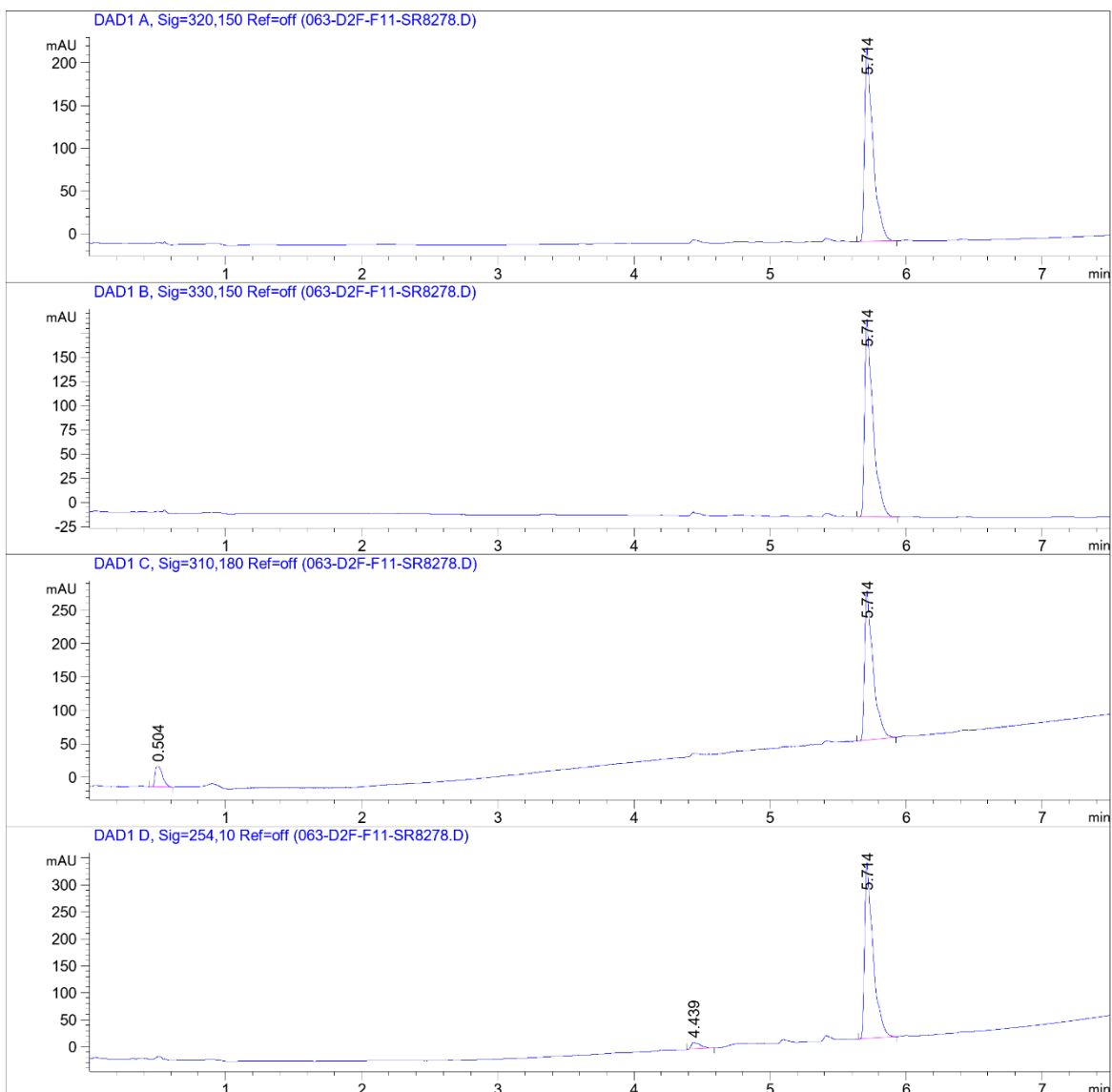
COMPOUND INFORMATION

Purity

Data File W:\analyti...PEN\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\063-D2F-F11-SR8278.D

Sample Name: SR8278

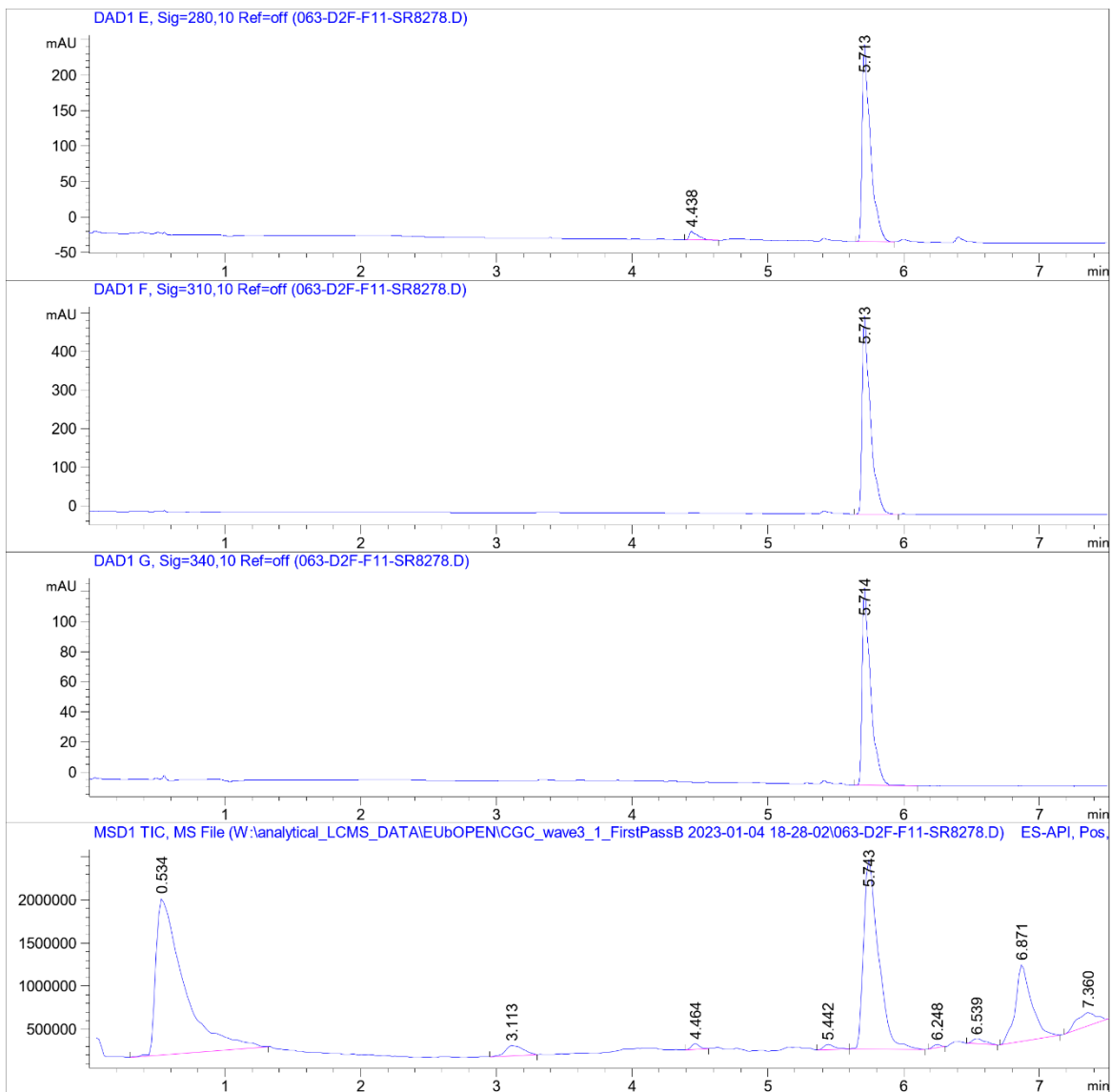
```
=====
Acq. Operator   : SYSTEM                      Seq. Line :   63
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2F-F11
Injection Date  : 1/5/2023 5:56:25 AM        Inj       :    1
                                           Inj Volume: Inj prog
Sequence File   : 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
=====
```



COMPOUND INFORMATION

Data File W:\analyti...PEN\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\063-D2F-F11-SR8278.D

Sample Name: SR8278



COMPOUND INFORMATION

Data File W:\analyti...PEN\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\063-D2F-F11-SR8278.D

Sample Name: SR8278

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	25976634	157.00 I
-	-	3.113	1076920	239.00 I 217.10 I
-	-	4.464	283100	510.30 I 378.00 I 170.90 I
-	-	5.442	356940	400.00 I 378.10 I
5.714	966	5.743	16697945	362.00 I
-	-	6.248	151152	228.20 I 137.10 I
-	-	6.539	391411	280.20 I
-	-	6.871	7415539	282.20 I
-	-	7.360	1630597	400.30 I 282.30 I

