

Rosiglitazone

CAS Registry No.: 122320-73-4

Formal Name: 5-(4-(2-(methyl(pyridin-2-yl)amino)ethoxy)benzyl)thiazolidine-2,4-dione

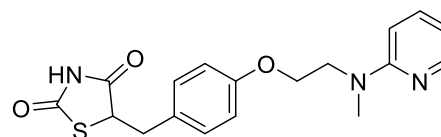
EUBOPEN ID: EUB0000190b

Molecular Formula: C₁₈H₁₉N₃O₃S

Molecular Weight: 357.43 g/mol

Smiles: CN(CCOC1=CC=C(C=C1)CC2C(=O)NC(=O)S2)C3=CC=CC=N3

Recommended concentration: 1 μM

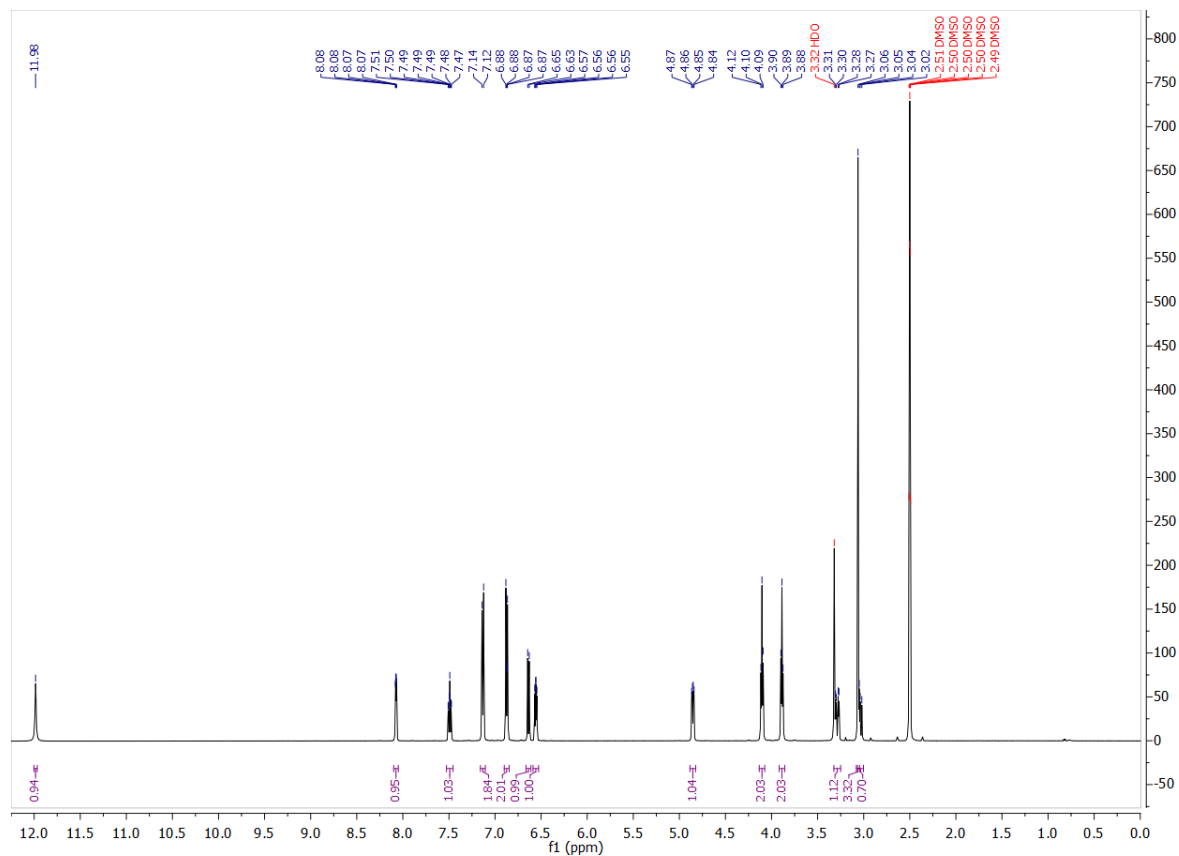


Biological activity

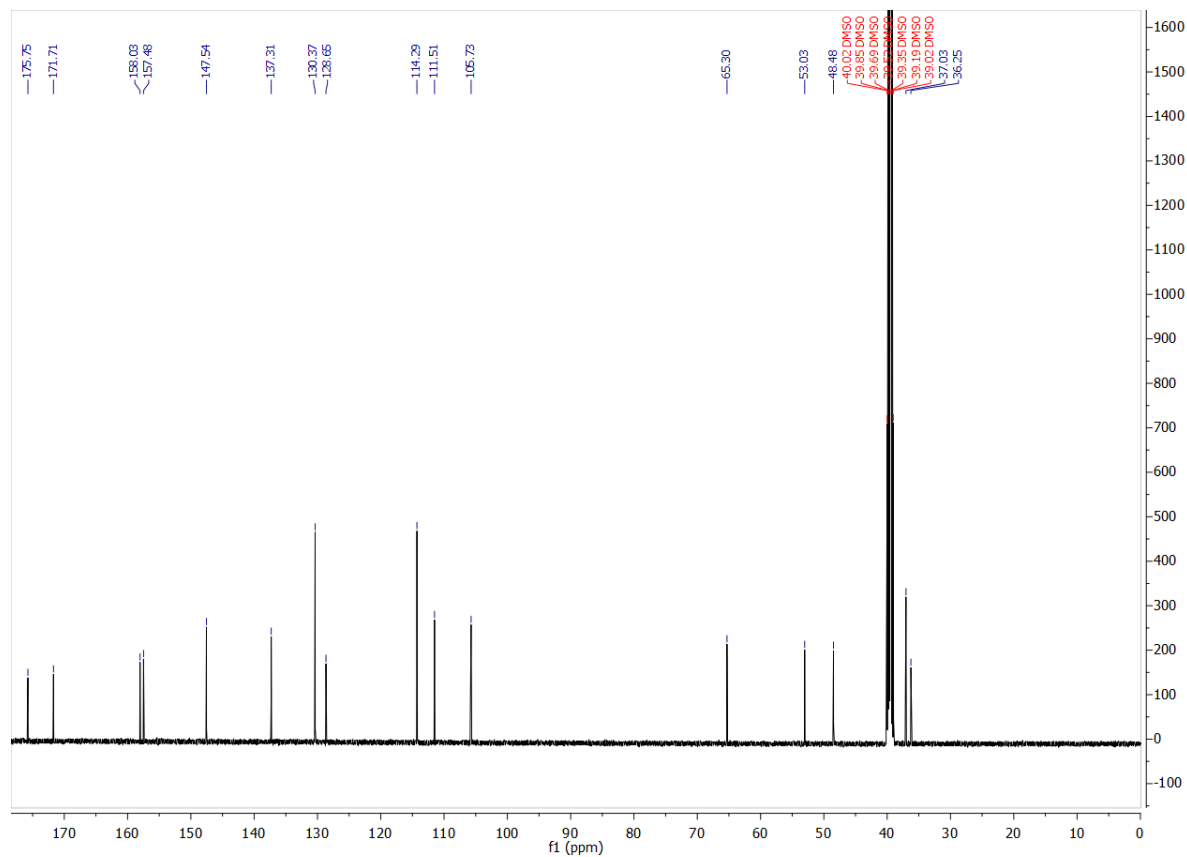
	Type	IC ₅₀ /EC ₅₀ [μM]	Reference
Main NR target:	NR1C3 (PPARγ) Agonist	0.035	https://doi.org/10.1016/j.bmcl.2010.02.071
NR off-target:			

Identity

¹H NMR



¹³C NMR



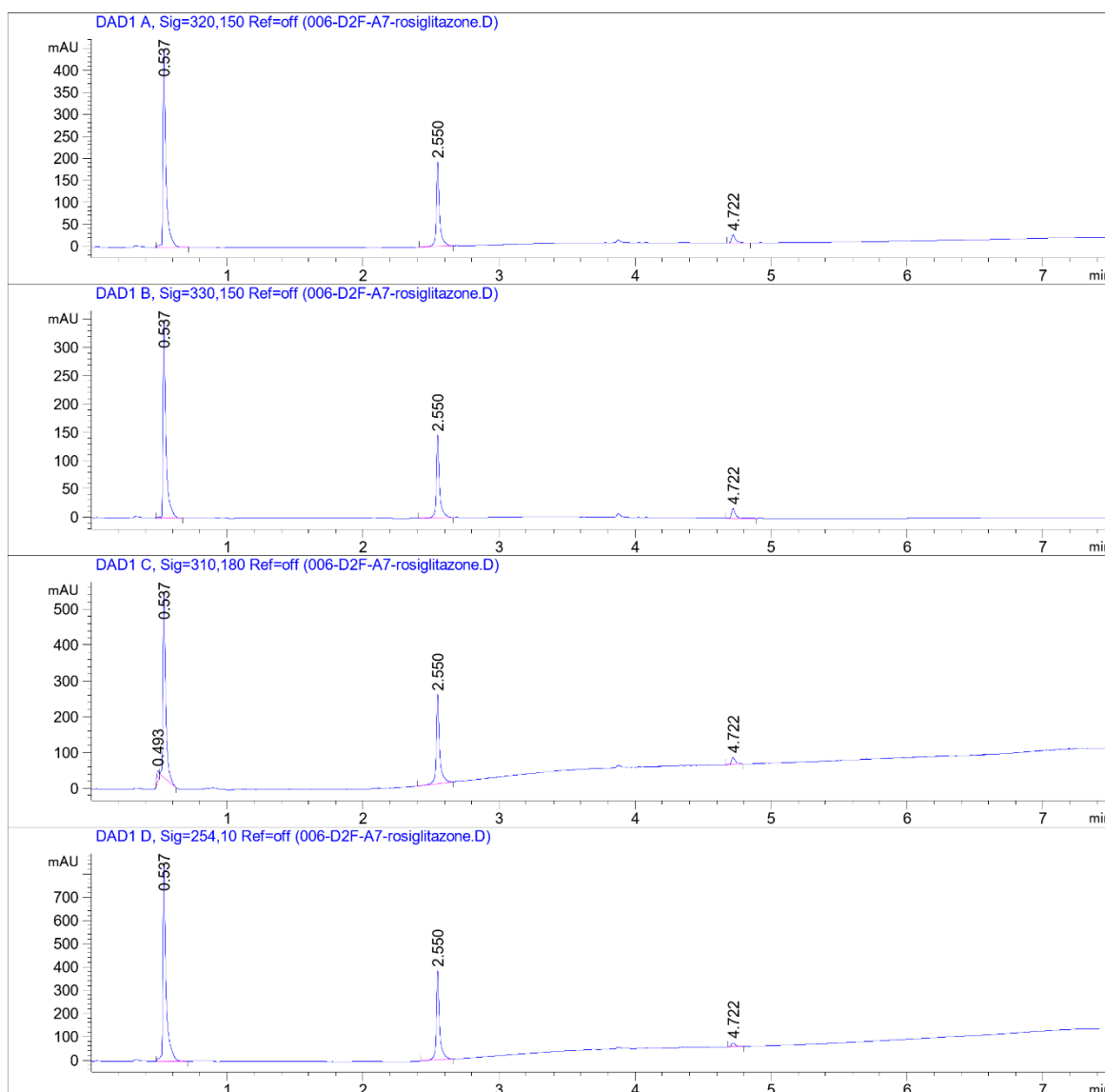
COMPOUND INFORMATION

Purity

Data File W:\analyti...C_ECH01-2_SecondPass 2021-03-23 18-53-53\006-D2F-A7-rosiglitazone.D

Sample Name: rosiglitazone

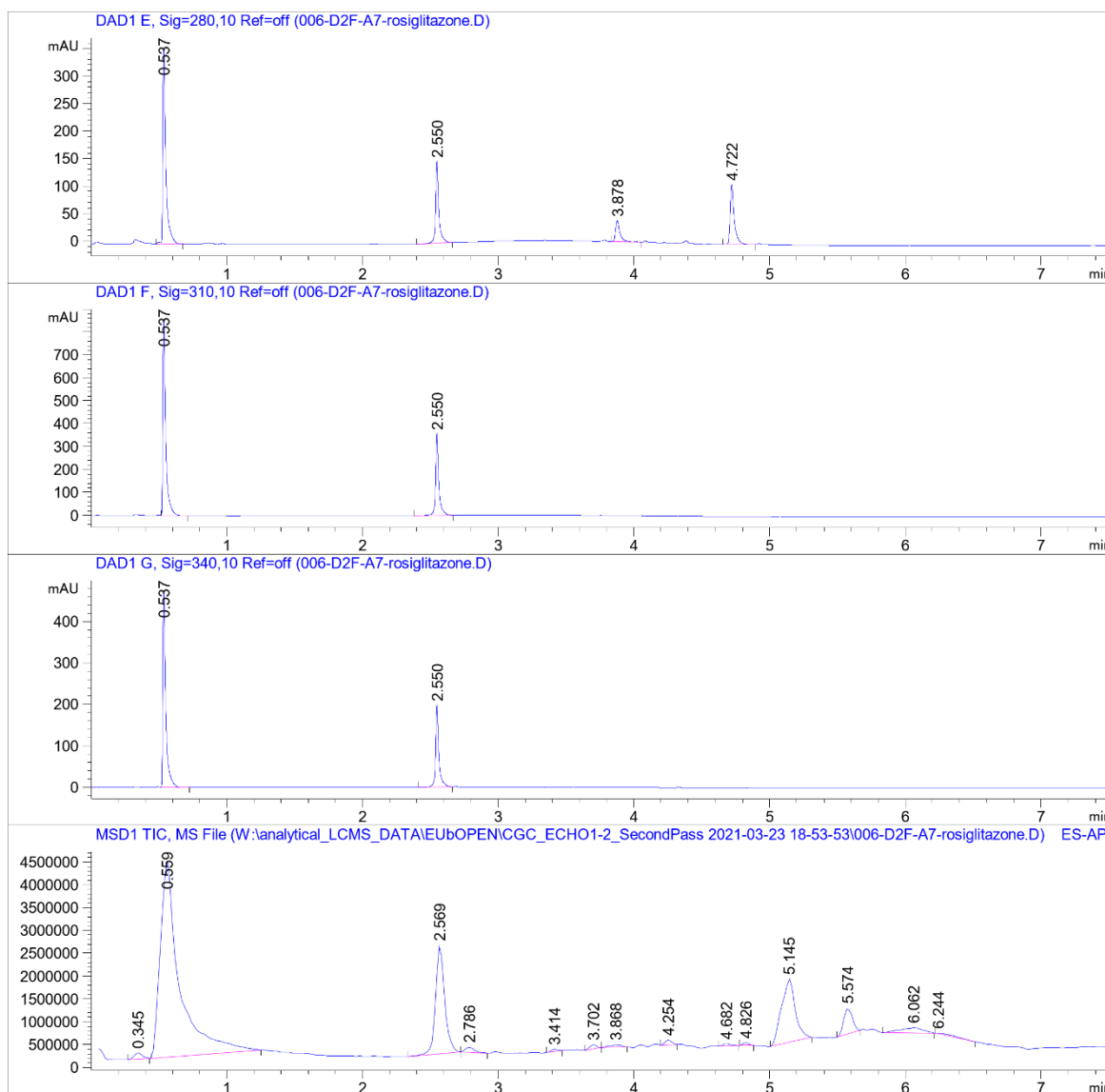
```
=====
Acq. Operator   : SYSTEM                      Seq. Line :    6
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2F-A7
Injection Date  : 3/23/2021 7:52:59 PM       Inj       :    1
                                           Inj Volume: Inj prog
Sequence File   : 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)
=====
```



COMPOUND INFORMATION

Data File W:\analyti...C_ECHO1-2_SecondPass 2021-03-23 18-53-53\006-D2F-A7-rosiglitazone.D

Sample Name: rosiglitazone



COMPOUND INFORMATION



Data File W:\analyti...C_ECHO1-2_SecondPass 2021-03-23 18-53-53\006-D2F-A7-rosiglitazone.D

Sample Name: rosiglitazone

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
-	-	0.345	574970	200.00 I 183.00 I 159.00 I 142.00 I 110.00 I
0.537	710	0.559	42584952	358.10 I
2.550	317	2.569	11259365	358.10 I
-	-	2.786	521762	217.10 I
-	-	3.414	182448	326.40 I
-	-	3.702	315982	312.20 I 214.10 I
-	-	3.868	324485	316.30 I 296.30 I 288.20 I 282.30 I 268.20 I 225.10 I 200.00 I 158.90 I 111.10 I 102.20 I
-	-	4.254	369752	296.30 I
4.722	37	4.682	192697	254.20 I
-	-	4.826	178529	280.30 I
-	-	5.145	9663870	282.30 I
-	-	5.574	2464099	359.30 I 341.30 I 284.30 I 282.30 I
-	-	6.062	1318681	282.20 I
-	-	6.244	278382	282.30 I

