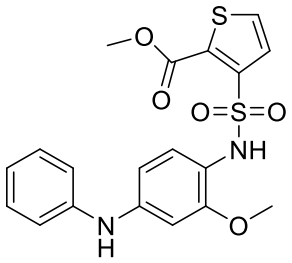
COMPOUND INFORMATION

GSK0660

CAS Registry No.:	1014691-61-2
Formal Name:	Methyl 3-(N-(2-methoxy-4-(phenylamino)phenyl)sulfamoyl)thiophene-2-carboxylate
EUbOPEN ID:	EUB0001150a
Molecular Formula:	$C_{19}H_{18}N_2O_5S_2$
Molecular Weight:	418.48 g/mol
Smiles:	COC1=C(C=CC(=C1)NC2=CC=CC=C2)NS(=O)(=O)C3=C(SC=C3)C(=O)OC
Recommended concentration:	10 µM



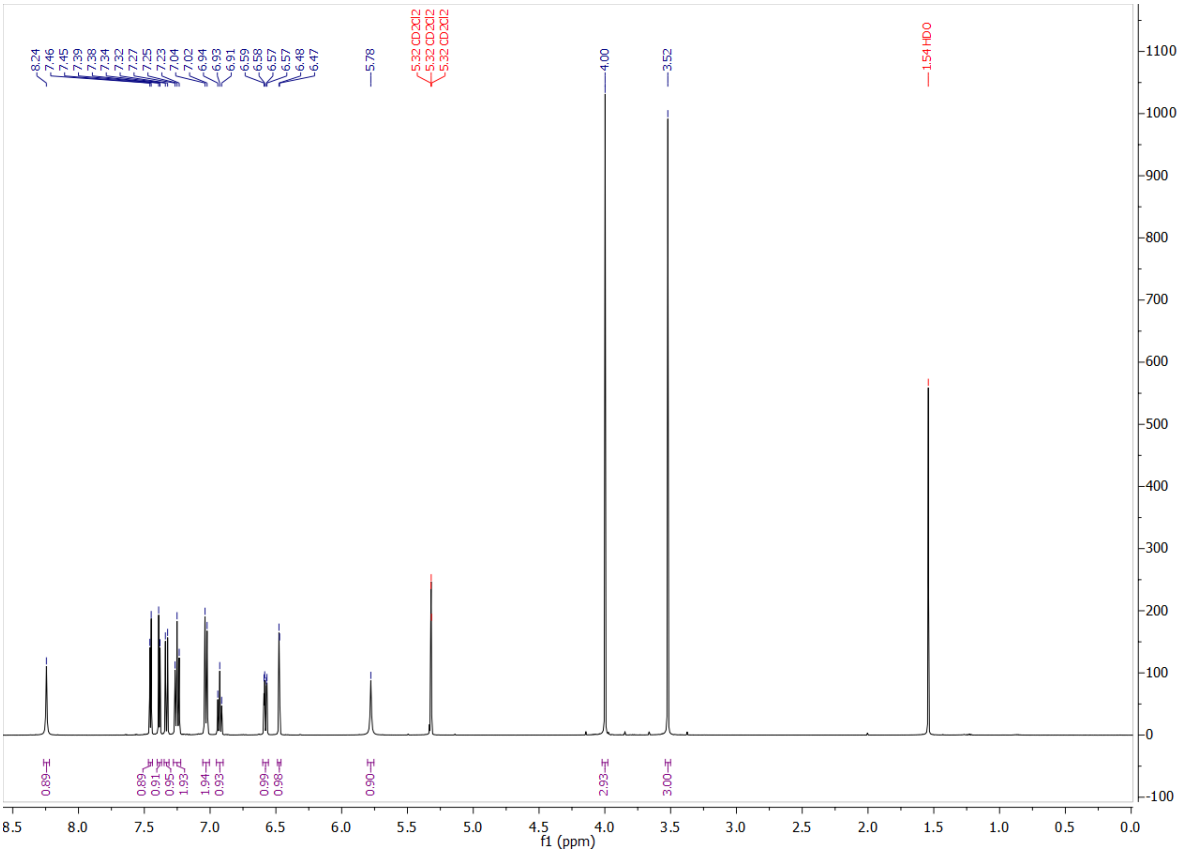
Biological activity

		Type	IC_{50}/EC_{50} [µM]	Reference
Main NR target:	NR1C1 (PPARα)	Antagonist	6.1	inhouse
	NR1C2 (PPARδ)	Antagonist	5.5	
	NR1C3 (PPARγ)	Antagonist	7.6	
NR off-target:				

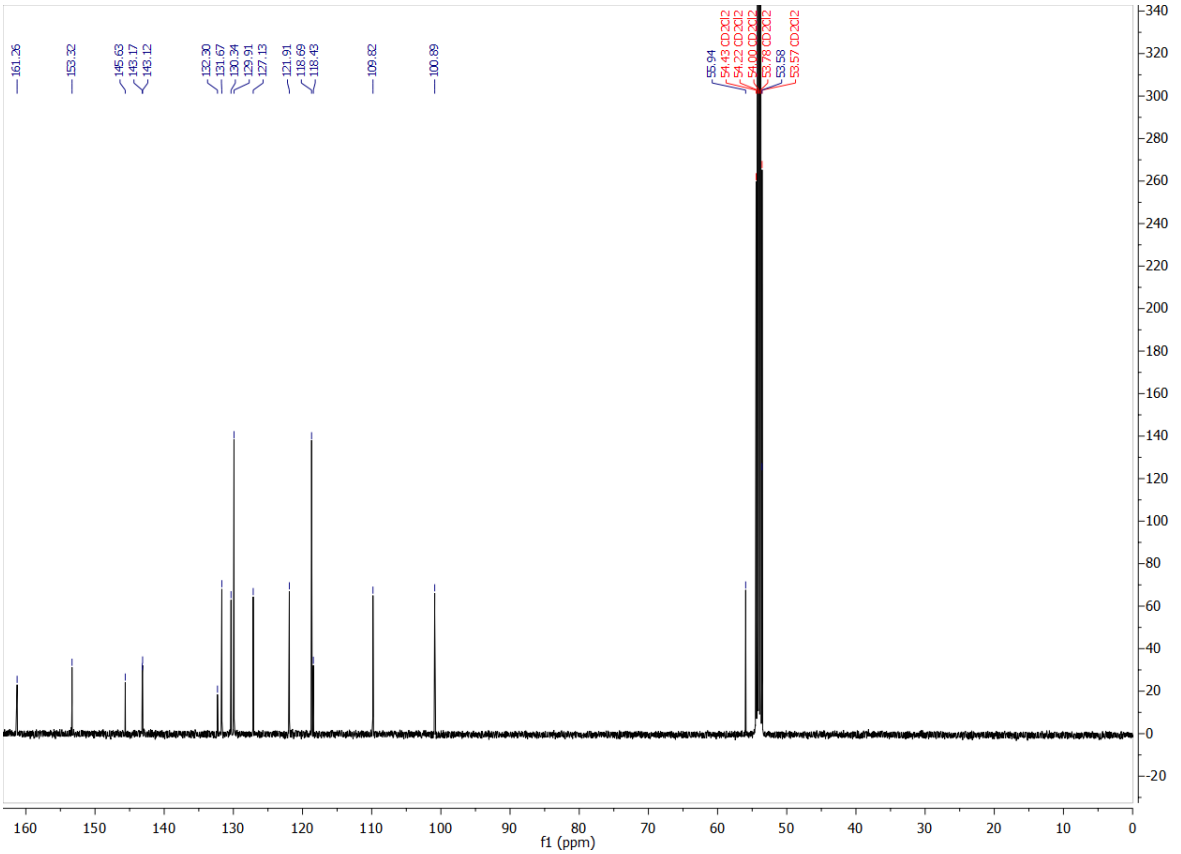
COMPOUND INFORMATION

Identity

^{1}H NMR



^{13}C NMR



COMPOUND INFORMATION

Purity

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Sample Name: GSK0660

```
======================================================================
Acq. Operator   : SYSTEM                        Seq. Line :  71
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                      Location :   D2F-F8
Injection Date  : 1/5/2023 7:24:53 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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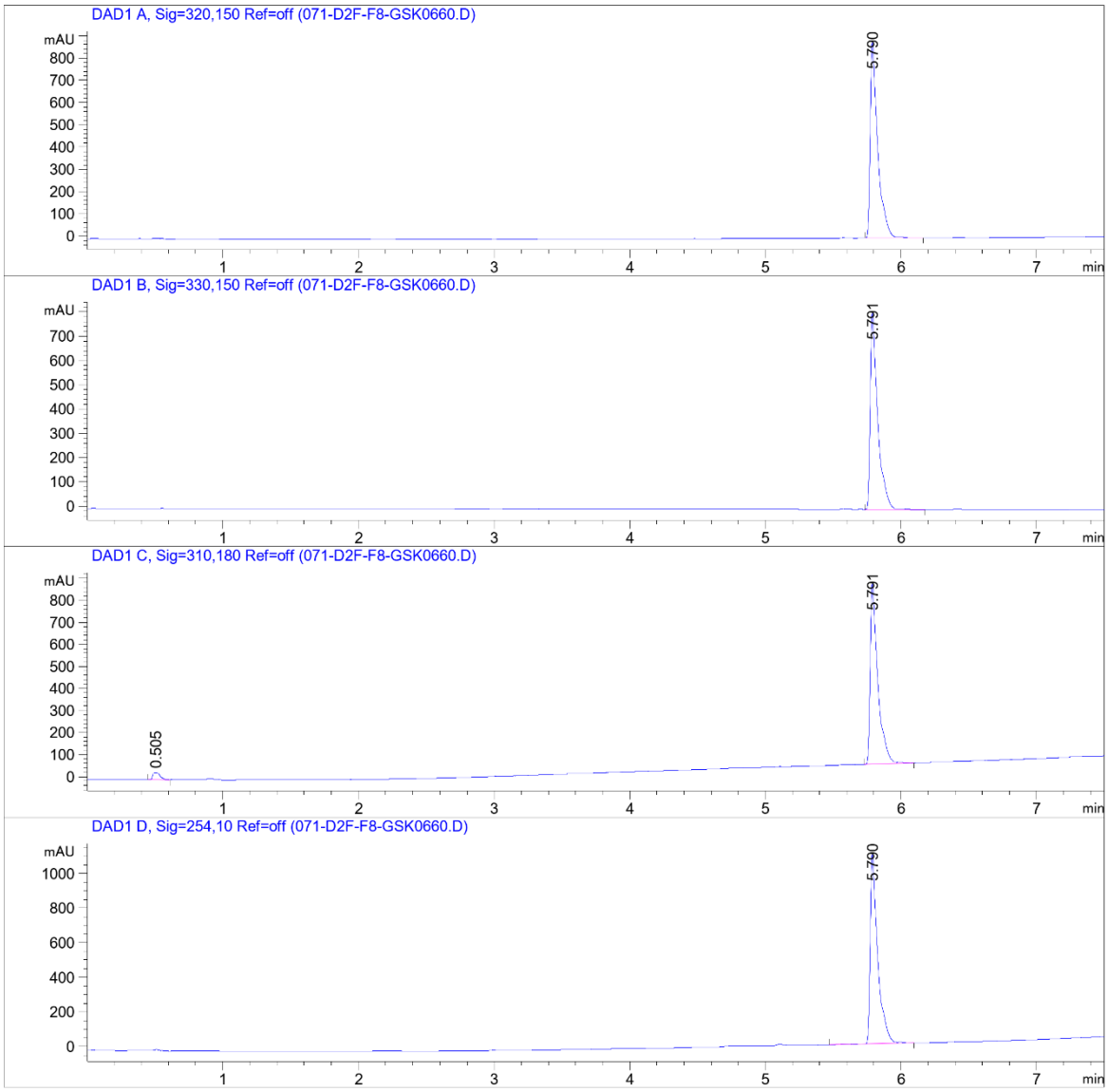
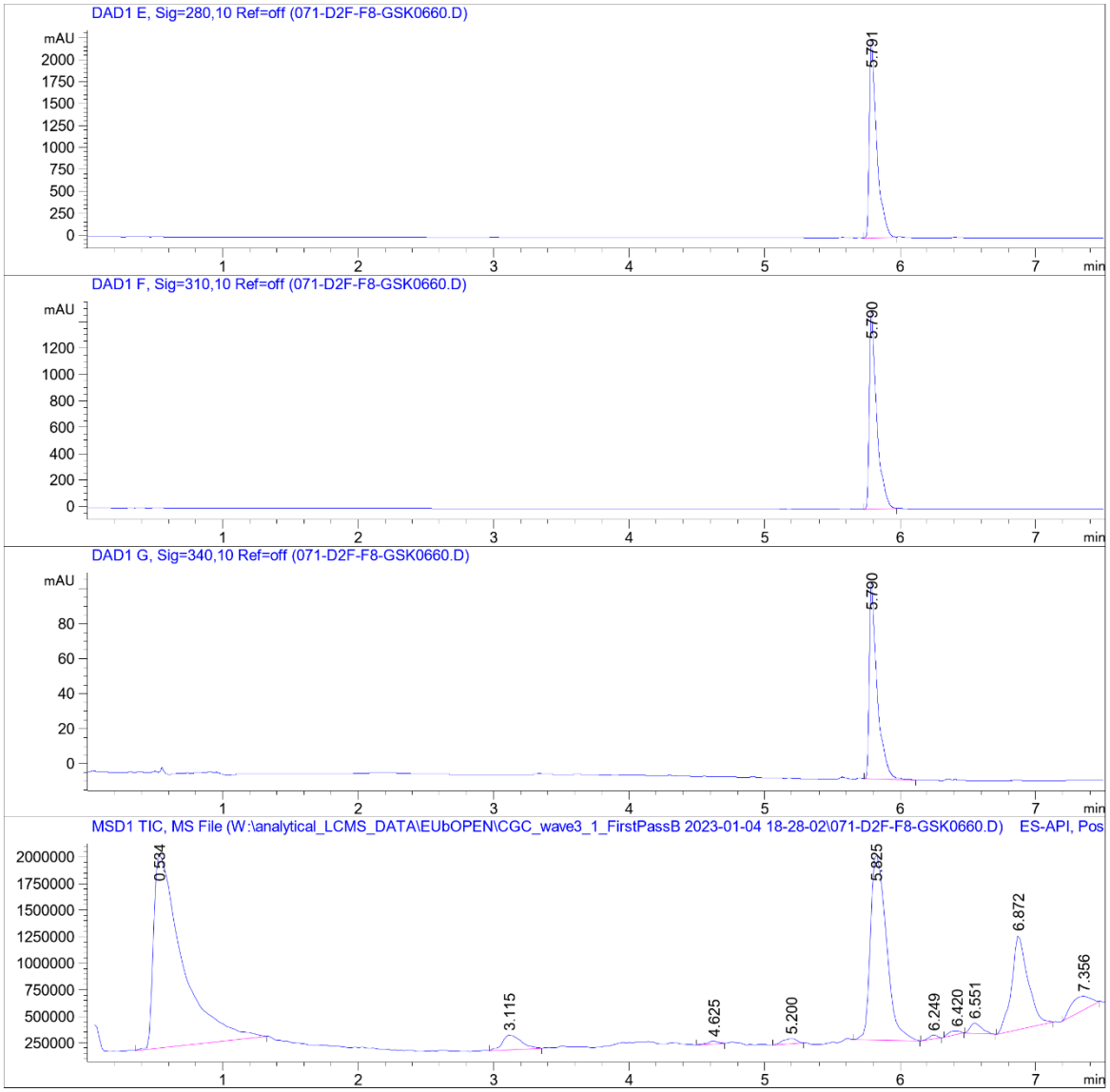


COMPOUND INFORMATION

Data File W:\analyti...PEN\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\071-D2F-F8-GSK0660.D
Sample Name: GSK0660

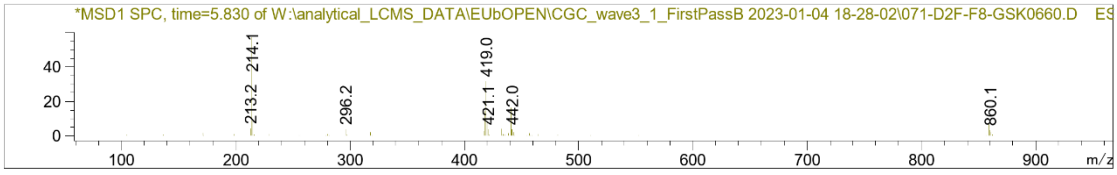


COMPOUND INFORMATION

Data File W:\analyti...PEN\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\071-D2F-F8-GSK0660.D
Sample Name: GSK0660

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	26793372	157.00 I
-	-	3.115	1309027	239.10 I
				217.10 I
-	-	4.625	145648	510.40 I
				170.80 I
				158.10 I
-	-	5.200	366719	510.40 I
				170.80 I
				137.10 I
5.790	3372	5.825	14282155	419.00 I
				214.10 I
-	-	6.249	154232	228.20 I
				137.10 I
-	-	6.420	214934	350.30 I
				282.30 I
				254.20 I
-	-	6.551	568204	507.30 I
				280.20 I
-	-	6.872	7399131	282.30 I
-	-	7.356	1385209	400.30 I
				282.30 I



Biological activity