

GSK2981278

CAS Registry No.: 1474110-21-8

Formal Name: N-(4-ethylphenyl)-3-(hydroxymethyl)-N-isobutyl-4-((tetrahydro-2H-pyran-4-yl)methoxy)benzenesulfonamide

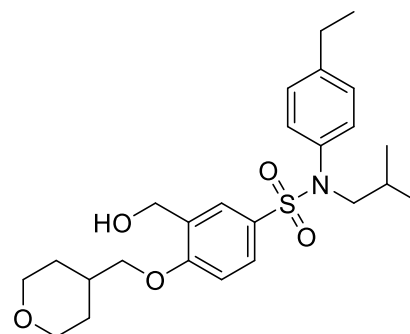
EUBOPEN ID: EUB0001159a

Molecular Formula: C₂₅H₃₅NO₅S

Molecular Weight: 461.62 g/mol

Smiles: OCC1=CC(S(N(C2=CC=C(C=C2)C)CC(C)C)(=O)=O)=CC=C1OCC3CCOCC3

Recommended concentration: 1 μM



Biological activity

		Type	IC ₅₀ /EC ₅₀ [μM]	Reference
Main NR target:	NR1F3 (RORγ)	inv. Agonist	0.02	https://doi.org/10.1016/j.bmcl.2018.03.041
NR off-target:				

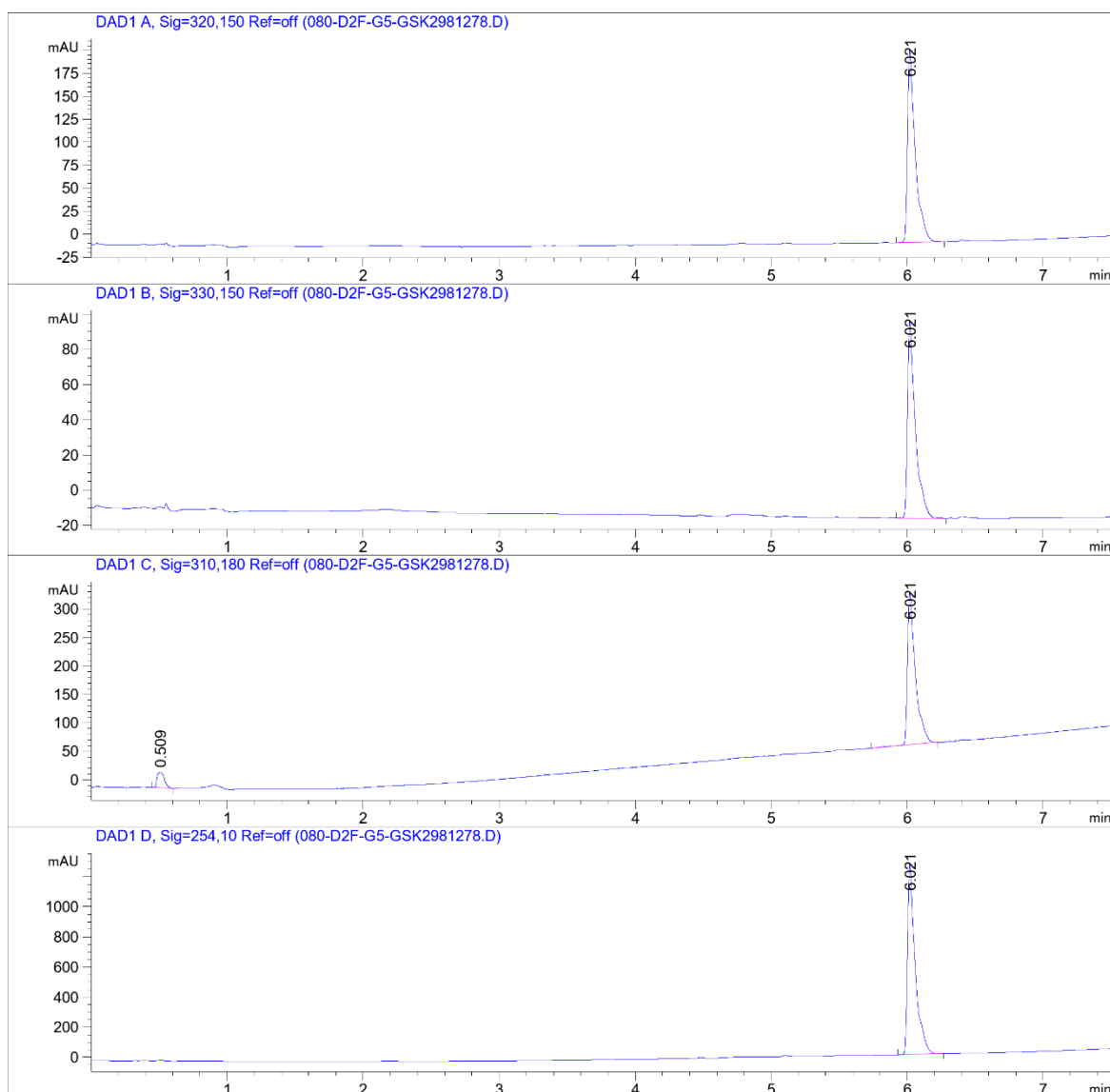
COMPOUND INFORMATION

Purity

Data File W:\analyti...\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\080-D2F-G5-GSK2981278.D

Sample Name: GSK2981278

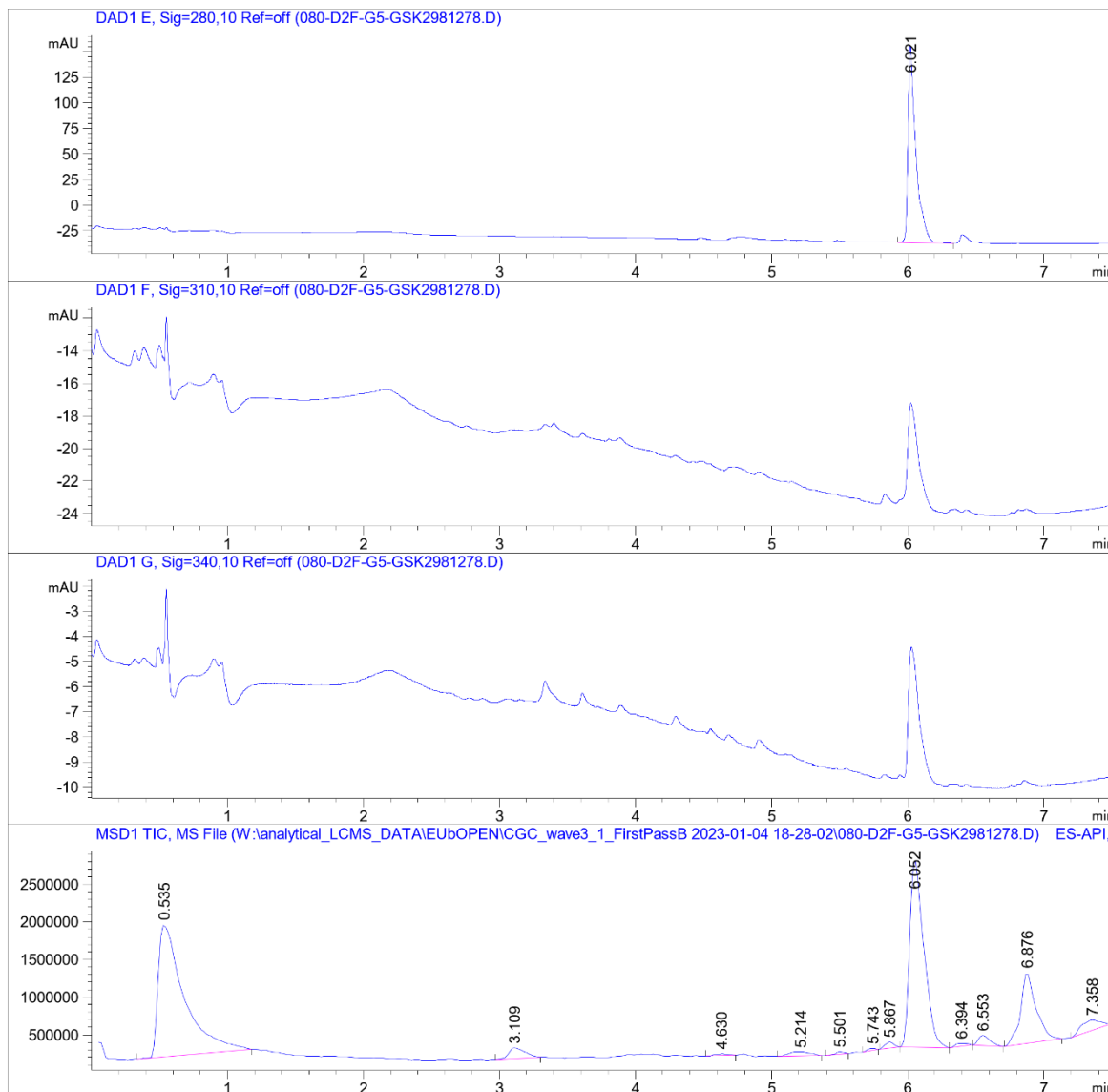
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=====
Acq. Operator   : SYSTEM                      Seq. Line :   80
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2F-G5
Injection Date  : 1/5/2023 9:04:24 AM        Inj       :    1
                                           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\080-D2F-G5-GSK2981278.D

Sample Name: GSK2981278



COMPOUND INFORMATION

Data File W:\analyti...\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\080-D2F-G5-GSK2981278.D

Sample Name: GSK2981278

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
-	-	0.535	23267944	157.00 I
-	-	3.109	1163551	239.10 I 217.10 I
-	-	4.630	149446	510.30 I 255.80 I 170.90 I 158.20 I 137.10 I
-	-	5.214	545907	510.40 I 338.20 I 336.20 I 316.30 I 170.90 I 137.10 I 105.10 I
-	-	5.501	113315	510.30 I 504.20 I 137.10 I 105.10 I
-	-	5.743	127128	280.20 I
-	-	5.867	365227	318.20 I 296.20 I
6.021	821	6.052	18098704	462.20 I
-	-	6.394	237599	254.20 I
-	-	6.553	784433	507.20 I 485.30 I 280.20 I
-	-	6.876	7492533	282.20 I
-	-	7.358	1335475	400.30 I 282.20 I

