

T0901317

CAS Registry No.: 293754-55-9

Formal Name: N-(4-(1,1,1,3,3,3-hexafluoro-2-hydroxypropan-2-yl)phenyl)-N-(2,2,2-trifluoroethyl)benzenesulfonamide

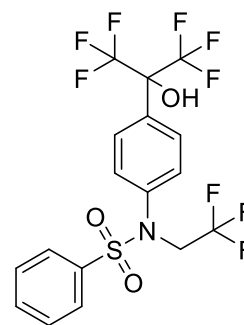
EUBOPEN ID: EUB0000040b

Molecular Formula: C₁₇H₁₂F₉NO₃S

Molecular Weight: 481.33 g/mol

Smiles: O=S(C1=CC=CC=C1)(N(C2=CC=C(C(C(F)(F)F)(O)C(F)(F)F)C=C2)CC(F)(F)F)=O

Recommended concentration: 1 μM

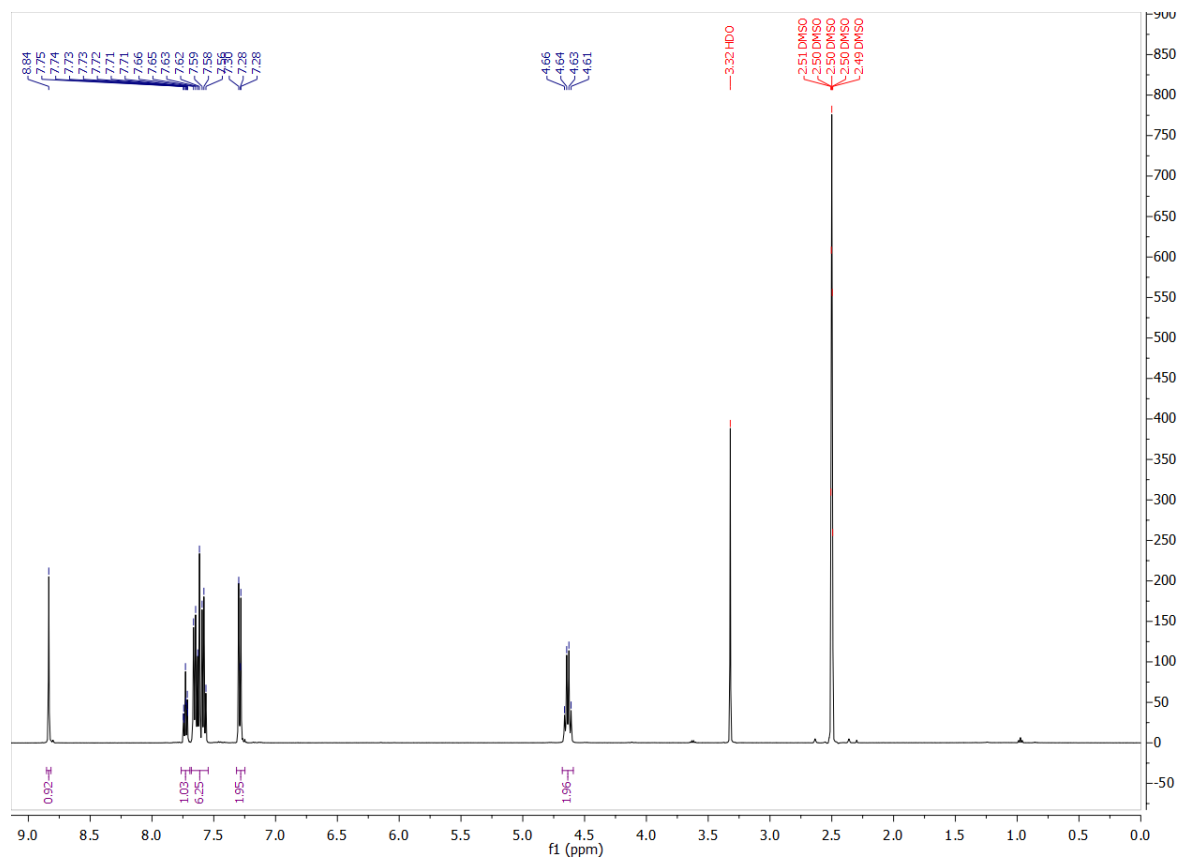


Biological activity

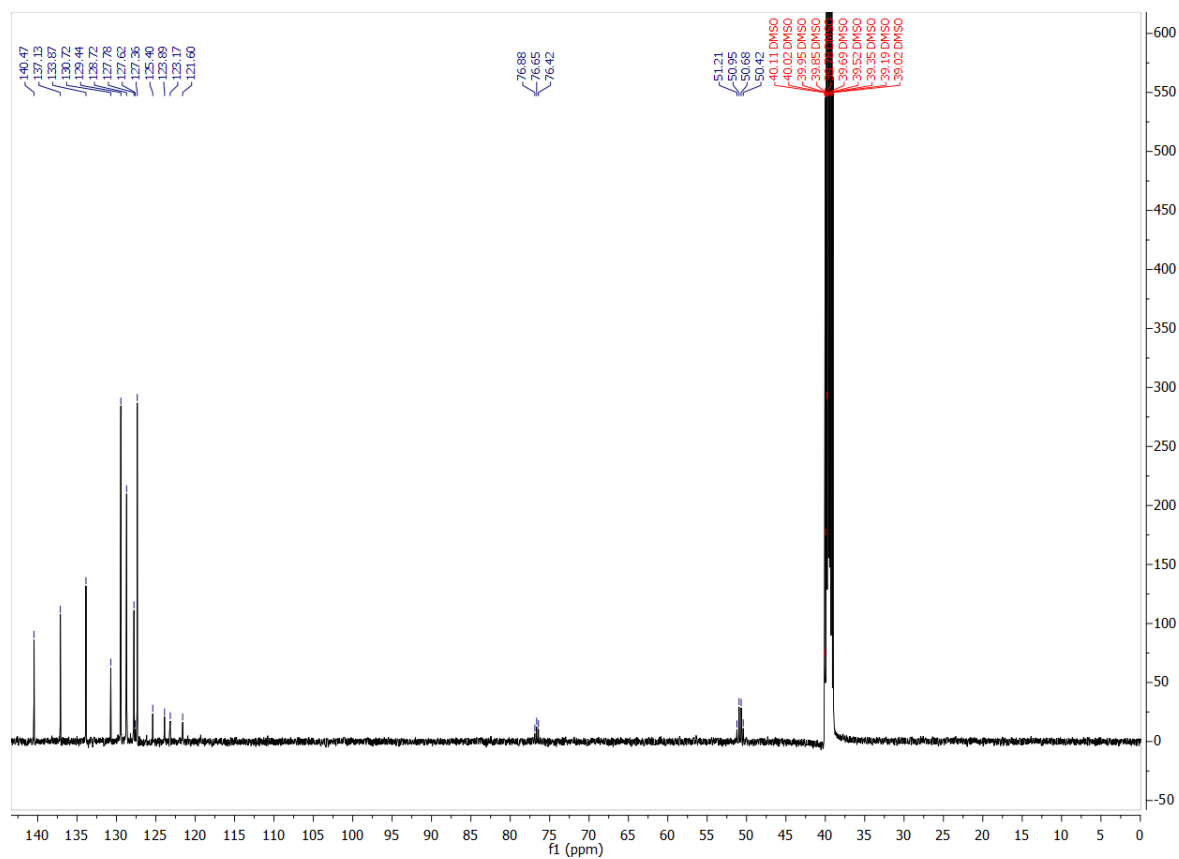
		Type	IC ₅₀ /EC ₅₀ [μM]	Reference
Main NR target:	NR1F3 (RORγ)	inv. Agonist	0.5	https://doi.org/10.1021/jm401901d
	NR1H3 (LXRα)	Agonist	0.4	
	NR1H2 (LXRβ)	Agonist	0.2	
	NR1I2 (PXR)	Agonist	0.04	
NR off-target:	NR1H4 (FXR)	Agonism	1.3	https://doi.org/10.1021/jm401901d

Identity

¹H NMR



¹³C NMR



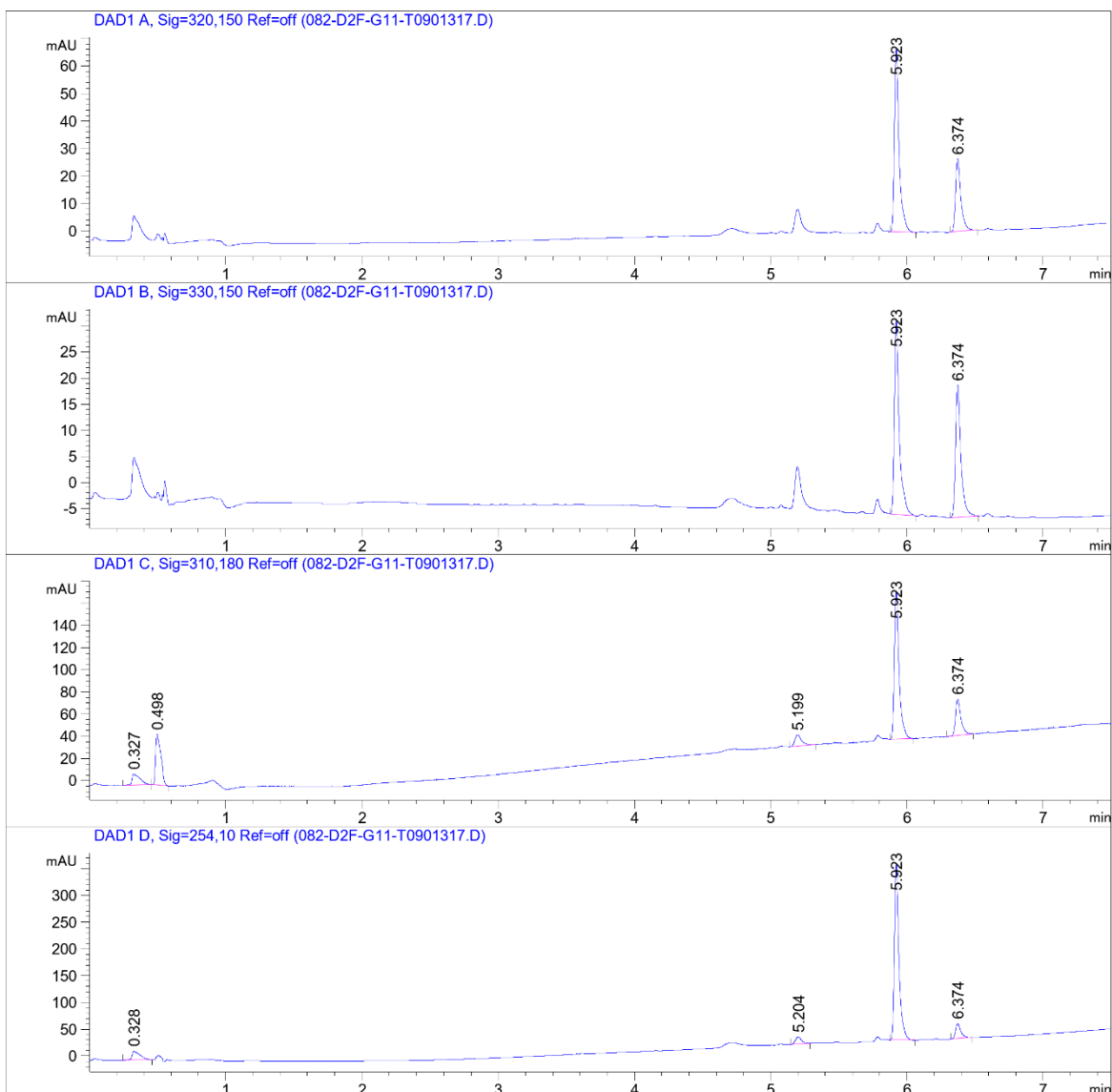
COMPOUND INFORMATION

Purity

Data File W:\analyti...\CGC_wave2_4_FirstPassB 2022-02-18 17-58-18\082-D2F-G11-T0901317.D

Sample Name: T0901317

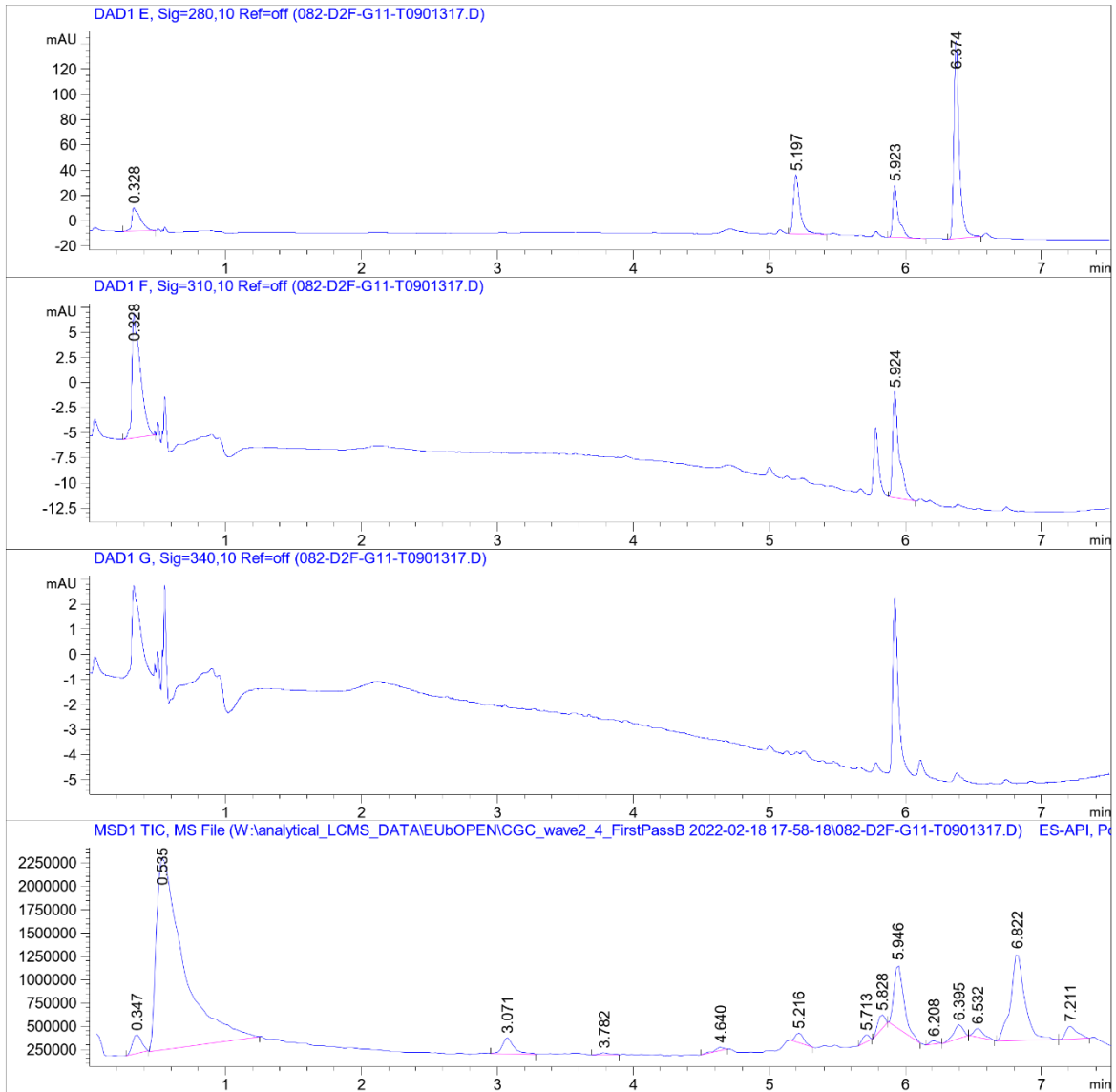
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=====
Acq. Operator   : SYSTEM                      Seq. Line :   82
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2F-G11
Injection Date  : 2/19/2022 8:56:50 AM       Inj       :    1
                                           Inj Volume: Inj prog
Sequence File   : W:\analytical_LCMS_DATA\EUBOPEN\CGC_wave2_4_FirstPassB 2022-02-18 17-58-18
                  \CGC_wave2_4_FirstPassB.S
Method          : W:\analytical_LCMS_DATA\EUBOPEN\CGC_wave2_4_FirstPassB 2022-02-18 17-58-18
                  \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...\N\CGC_wave2_4_FirstPassB 2022-02-18 17-58-18\082-D2F-G11-T0901317.D

Sample Name: T0901317



COMPOUND INFORMATION



Data File W:\analyti...\N\CGC_wave2_4_FirstPassB 2022-02-18 17-58-18\082-D2F-G11-T0901317.D

Sample Name: T0901317

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
-	-	0.347	917991	199.90 I 182.90 I 158.90 I 158.00 I 141.90 I 101.00 I
-	-	0.535	28780390	157.00 I
-	-	3.071	989882	239.00 I 217.00 I
-	-	3.782	116894	274.20 I
-	-	4.640	176651	332.20 I
-	-	5.216	454801	338.20 I 316.20 I
-	-	5.713	251208	280.20 I
-	-	5.828	547018	318.20 I 296.20 I
5.923	161	5.946	3399445	482.00 I
-	-	6.208	146868	228.10 I
6.374	72	6.395	700252	350.30 I 282.20 I 254.20 I 243.00 I
-	-	6.532	449043	507.20 I 485.20 I 280.20 I
-	-	6.822	6657310	282.20 I
-	-	7.211	806416	284.20 I 282.20 I

