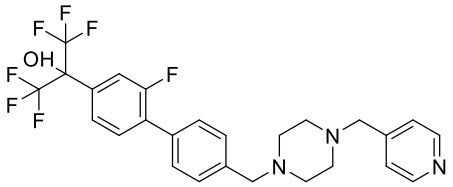
COMPOUND INFORMATION

SR2211

CAS Registry No.:	1359164-11-6
Formal Name:	1,1,1,3,3,3-hexafluoro-2-(2-fluoro-4'-((4-(pyridin-4-ylmethyl)piperazin-1-yl)methyl)-[1,1'-biphenyl]-4-yl)propan-2-ol
EUBOPEN ID:	EUB0001160a
Molecular Formula:	$C_{26}H_{24}F_7N_3O$
Molecular Weight:	527.49 g/mol
Smiles:	FC1=C(C2=CC=C(CN3CCN(CC4=CC=NC=C4)CC3)C=C2)C=CC(C(C(F)(F)F)(O)C(F)(F)F)=C1
Recommended concentration:	1 µM



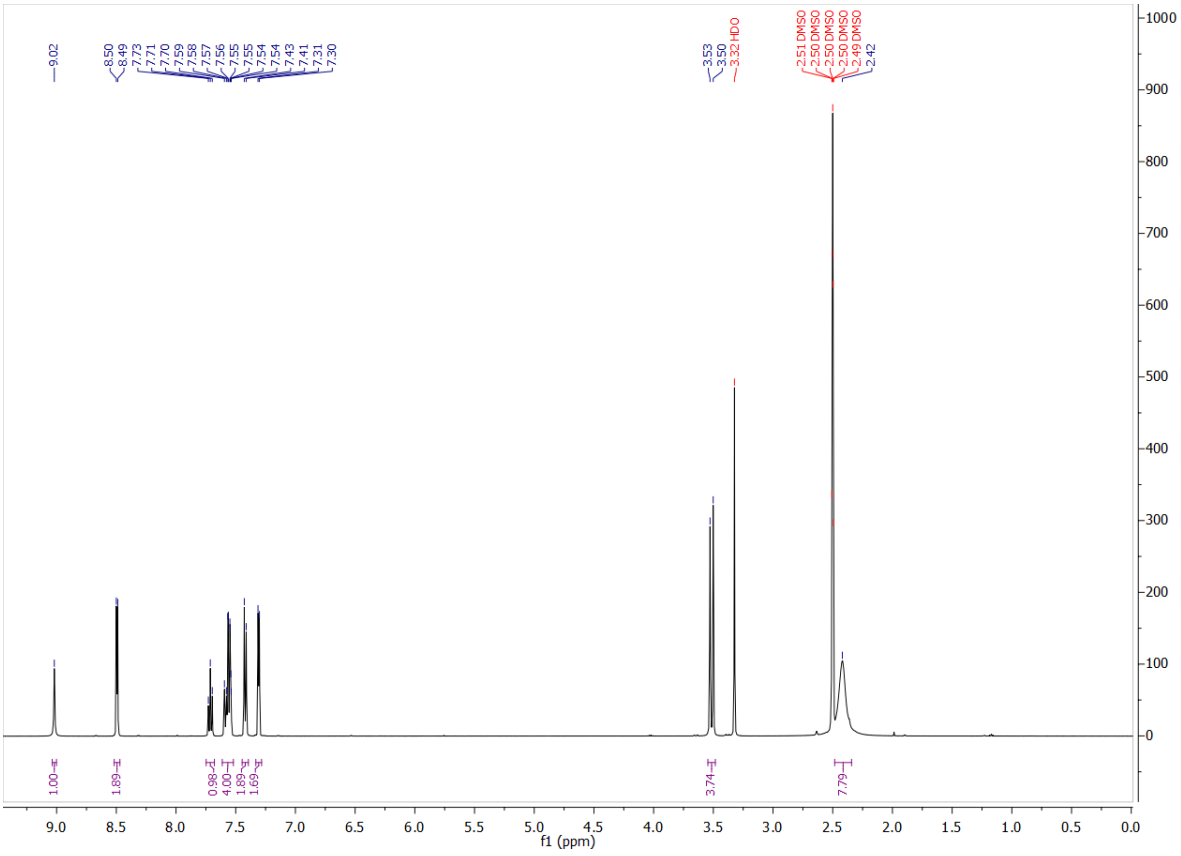
Biological activity

		Type	IC_{50}/EC_{50} [µM]	Reference
Main NR target:	NR1F3 (RORγ)	inv. Agonist	0.3	https://doi.org/10.1021/cb200496y
NR off-target:				

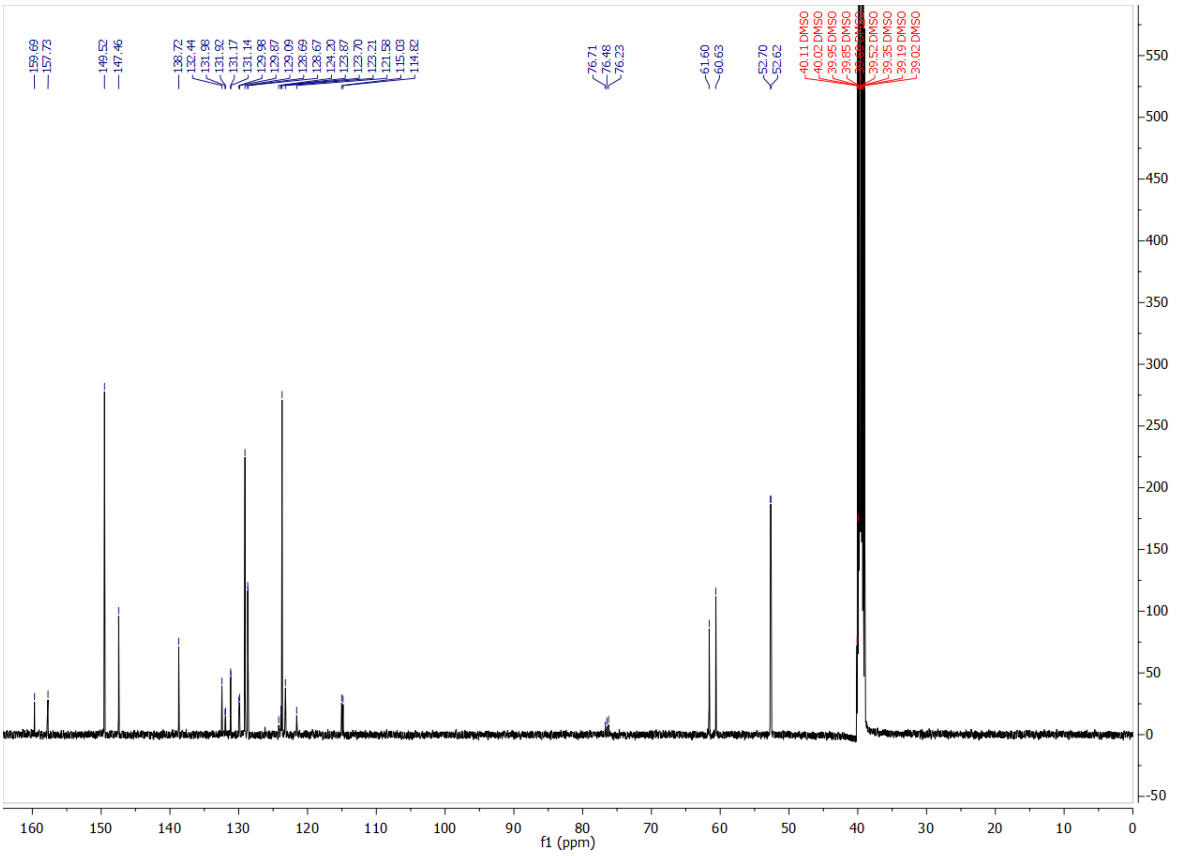
COMPOUND INFORMATION

Identity

^{1}H NMR



^{13}C NMR



COMPOUND INFORMATION

Purity

Data File W:\analyti...OPEN\CGC_wave3_3rdrun_vials 2023-04-14 23-47-17\004-D1F-B4-SR2211.D
Sample Name: SR2211

```
======================================================================
Acq. Operator   : SYSTEM                          Seq. Line :   4
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                        Location :   D1F-B4
Injection Date  : 4/15/2023 12:24:54 AM                Inj :   1
                                                 Inj Volume : Inj prog
Sequence File   : W:\analytical_LCMS_DATA\EUbOPEN\CGC_wave3_3rdrun_vials 2023-04-14 23-47-17
                  \CGC_wave3_3rdrun_vials.S
Method          : W:\analytical_LCMS_DATA\EUbOPEN\CGC_wave3_3rdrun_vials 2023-04-14 23-47-17
                  \CGL_FIRSTPASS_GENERALMETHOD_VIAL1+2_VIAL_20220414.M (Sequence Method)
Last changed    : 4/14/2023 5:08:13 PM by SYSTEM
Method Info     : CGL wellplate, 0.5 uL of 10 mM DMSO, general method
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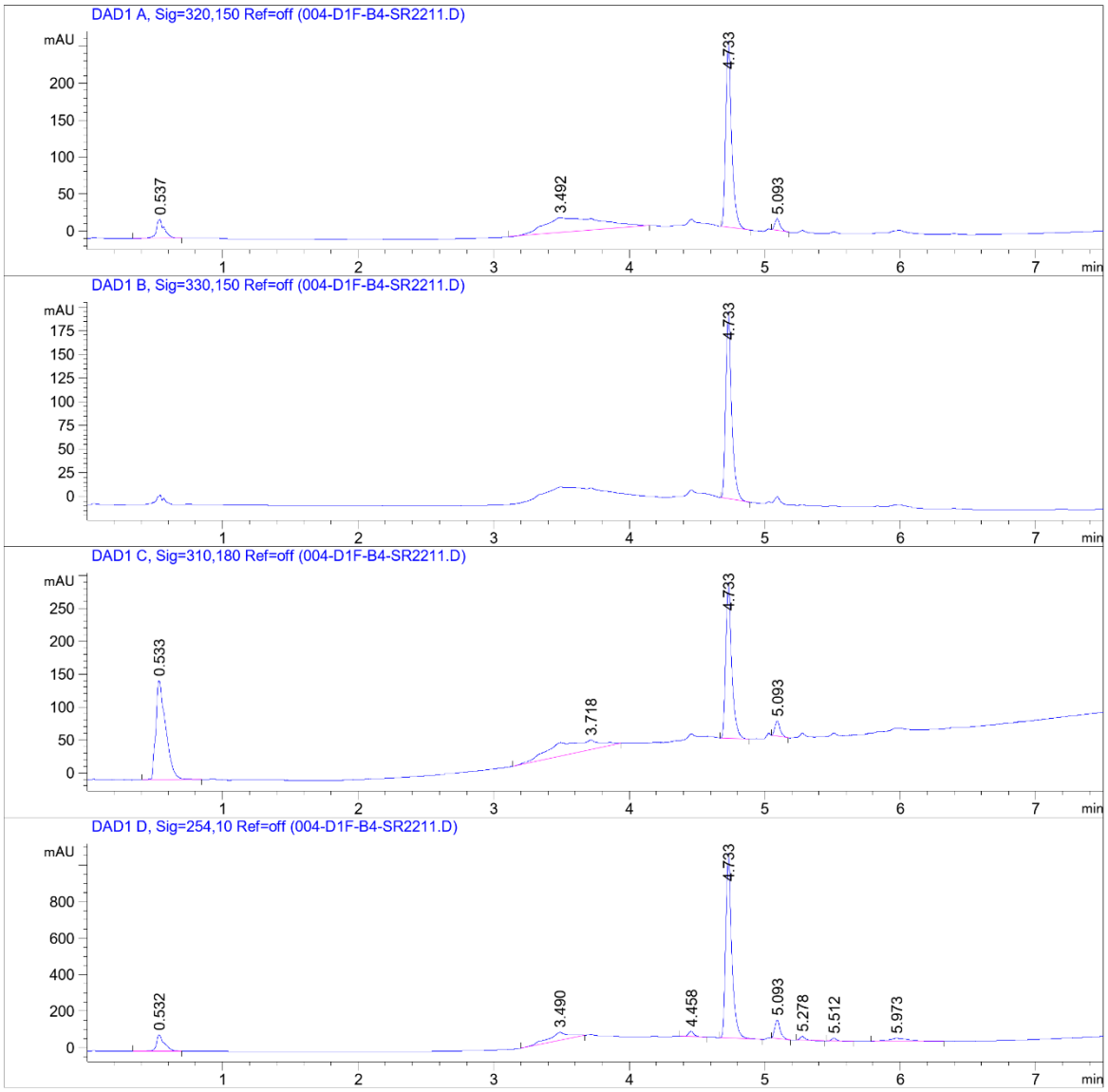
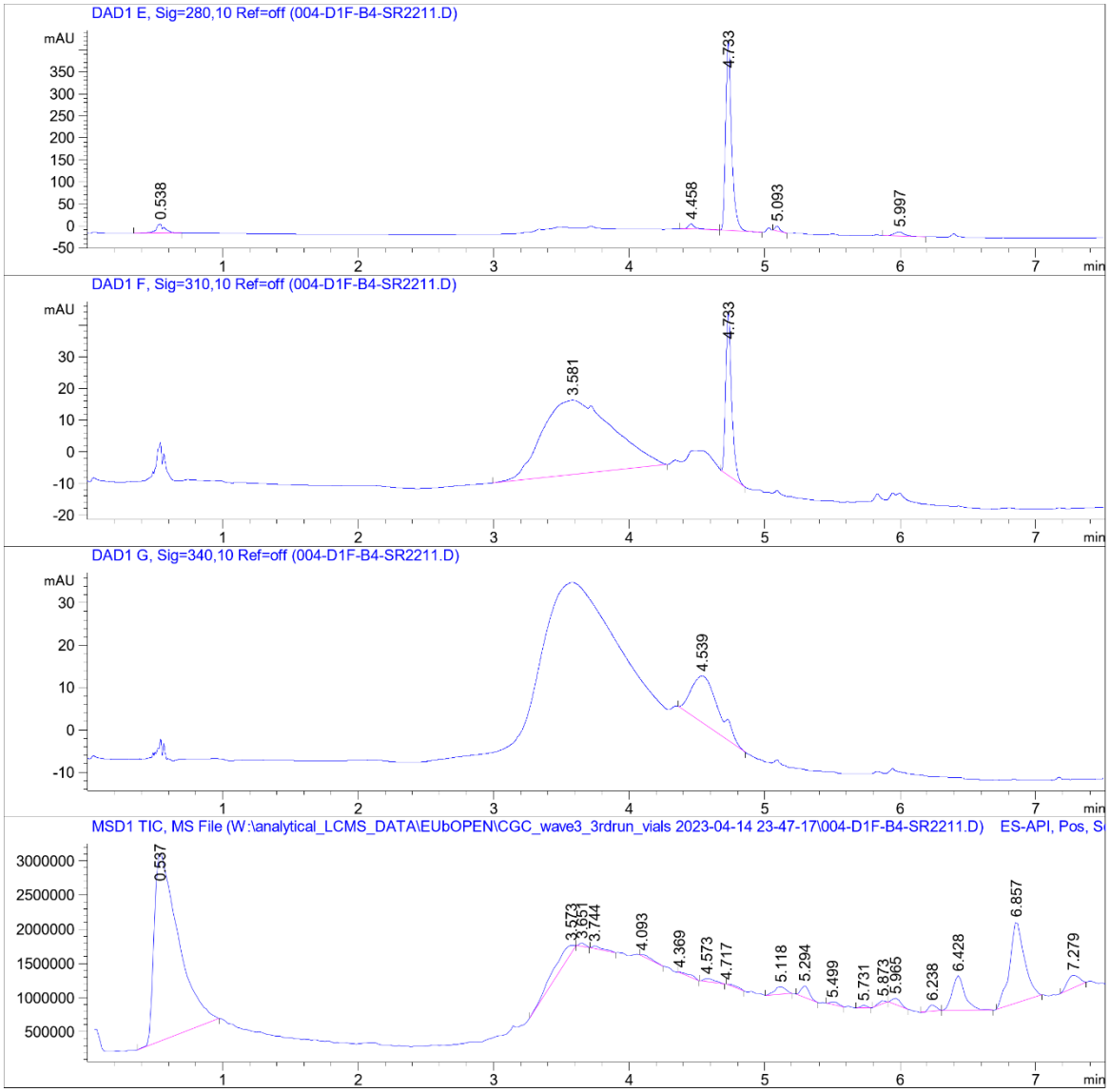


COMPOUND INFORMATION

Data File W:\analyti...OPEN\CGC_wave3_3rdrun_vials 2023-04-14 23-47-17\004-D1F-B4-SR2211.D
Sample Name: SR2211



COMPOUND INFORMATION

Data File W:\analyti...OPEN\CGC_wave3_3rdrun_vials 2023-04-14 23-47-17\004-D1F-B4-SR2211.D
Sample Name: SR2211

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
0.537	104	0.537	33914356	157.00 I
3.492	593	-	-	
-	-	3.573	2327656	170.80 I
-	-	3.651	162640	170.80 I
-	-	3.744	235333	170.80 I
-	-	4.093	197062	170.80 I
-	-	4.369	213335	170.80 I
-	-	4.573	273748	528.20 I 351.00 I 264.60 I 178.10 I 170.80 I
4.733	763	4.717	127689	528.20 I 351.00 I 264.60 I 178.10 I 170.80 I
5.093	43	5.118	606200	528.20 I 351.00 I 264.60 I 178.10 I
-	-	5.294	698966	528.20 I 398.20 I 376.20 I 351.00 I 264.60 I 178.10 I
-	-	5.499	181000	528.20 I 351.00 I 264.60 I 178.10 I
-	-	5.731	112807	528.10 I 351.00 I 280.20 I 264.60 I 178.10 I
-	-	5.873	152922	318.20 I 296.20 I
-	-	5.965	390011	528.20 I 282.20 I
-	-	6.238	359780	280.20 I 228.20 I

COMPOUND INFORMATION

-	-	6.428	3248994	350.20 I
				282.20 I
-	-	6.857	9042897	282.20 I
-	-	7.279	1142228	400.30 I
				284.30 I
				282.20 I