

COMPOUND INFORMATION

PF-06747711

CAS Registry No.: 1892576-58-7

Formal Name: 3-cyano-N-(3-(1-isobutrylpiperidin-4-yl)-1-methyl-4-(trifluoromethyl)-1H-pyrrolo[2,3-b]pyridin-5-yl)benzamide

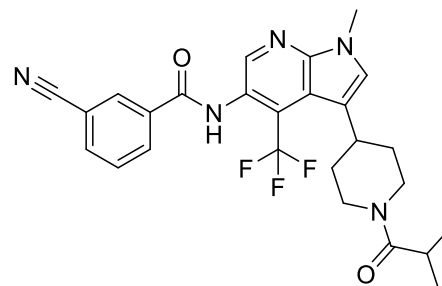
EUBOPEN ID: EUB0001170a

Molecular Formula: C₂₆H₂₆F₃N₅O₂

Molecular Weight: 497.52 g/mol

Smiles: FC(C1=C(NC(C2=CC(C#N)=CC=C2)=O)C=NC3=C1C(C4CCN(C(C)C)C)=O)CC4)=CN3C)(F)F

Recommended concentration: 1 μM



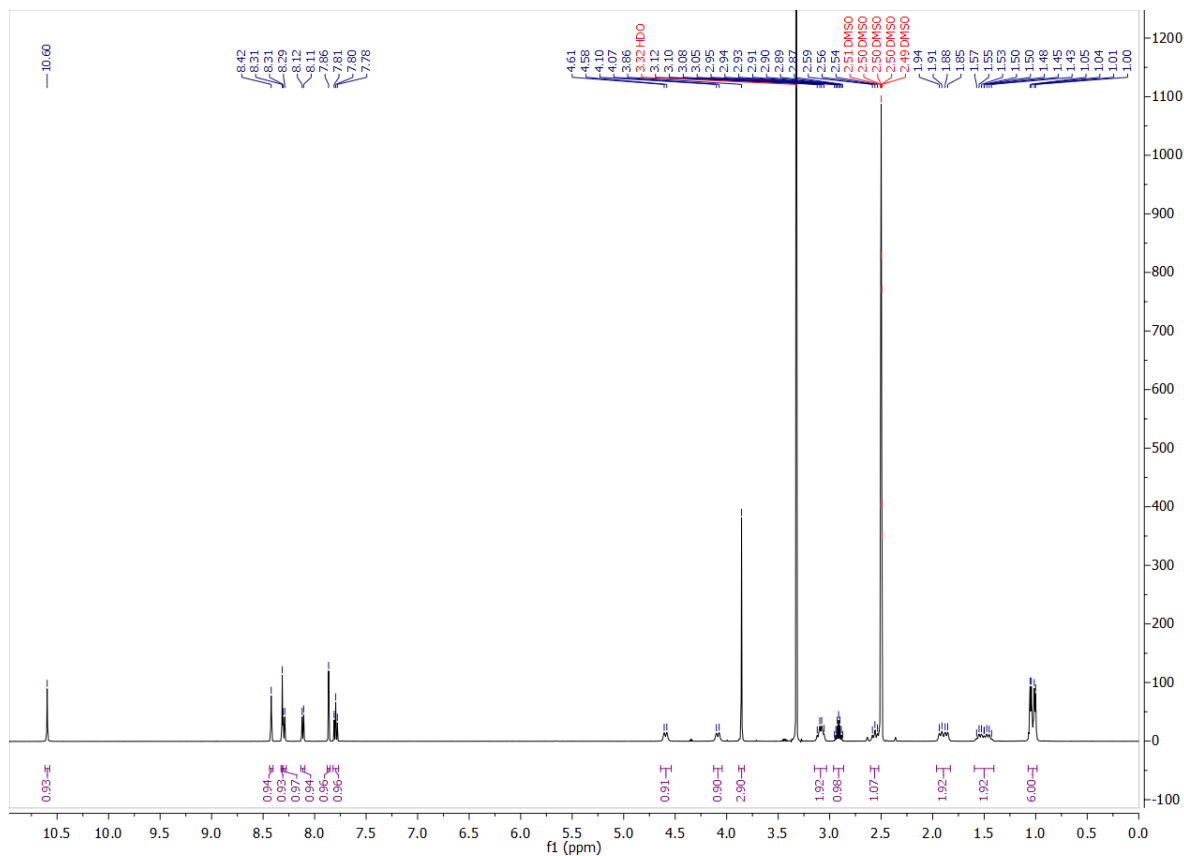
Biological activity

		Type	IC ₅₀ /EC ₅₀ [μM]	Reference
Main NR target:	NR1F3 (RORγ)	inv. Agonist	0.004	https://doi.org/10.1021/acs.jmedchem.8b00392
NR off-target:				

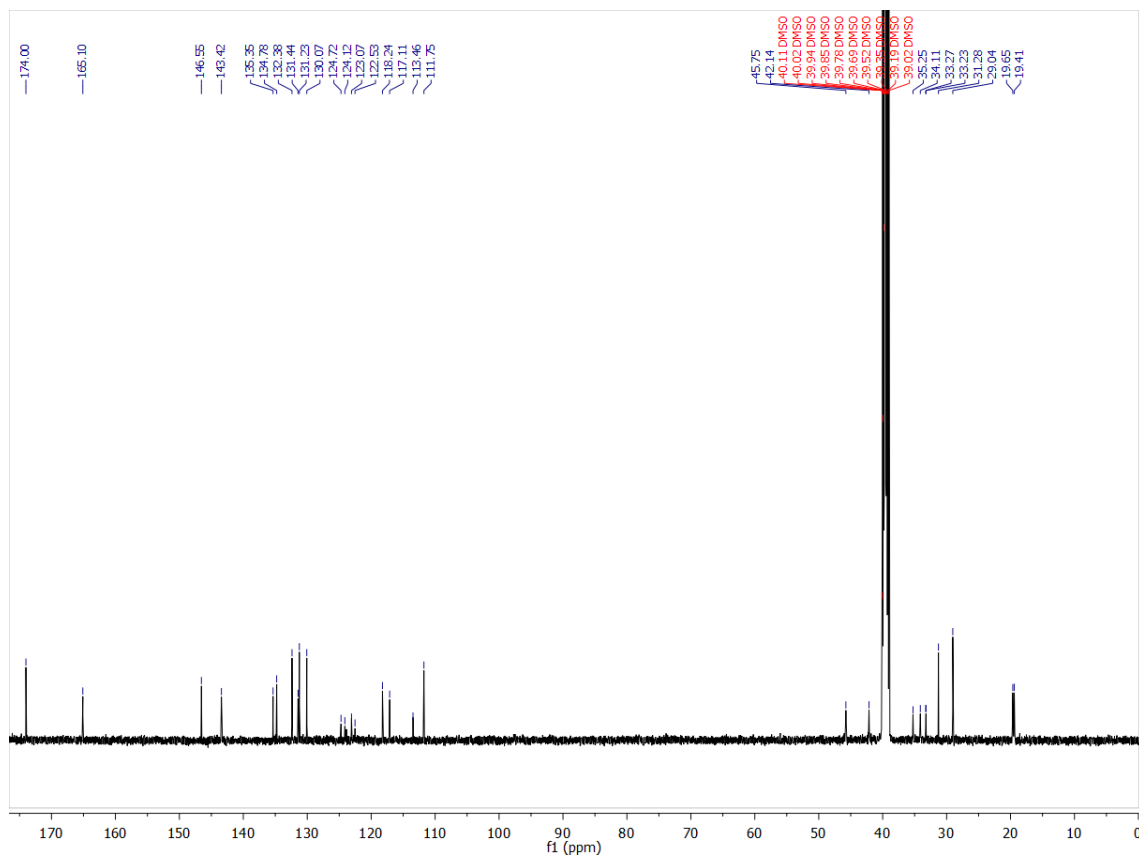
COMPOUND INFORMATION

Identity

¹H NMR



¹³C NMR



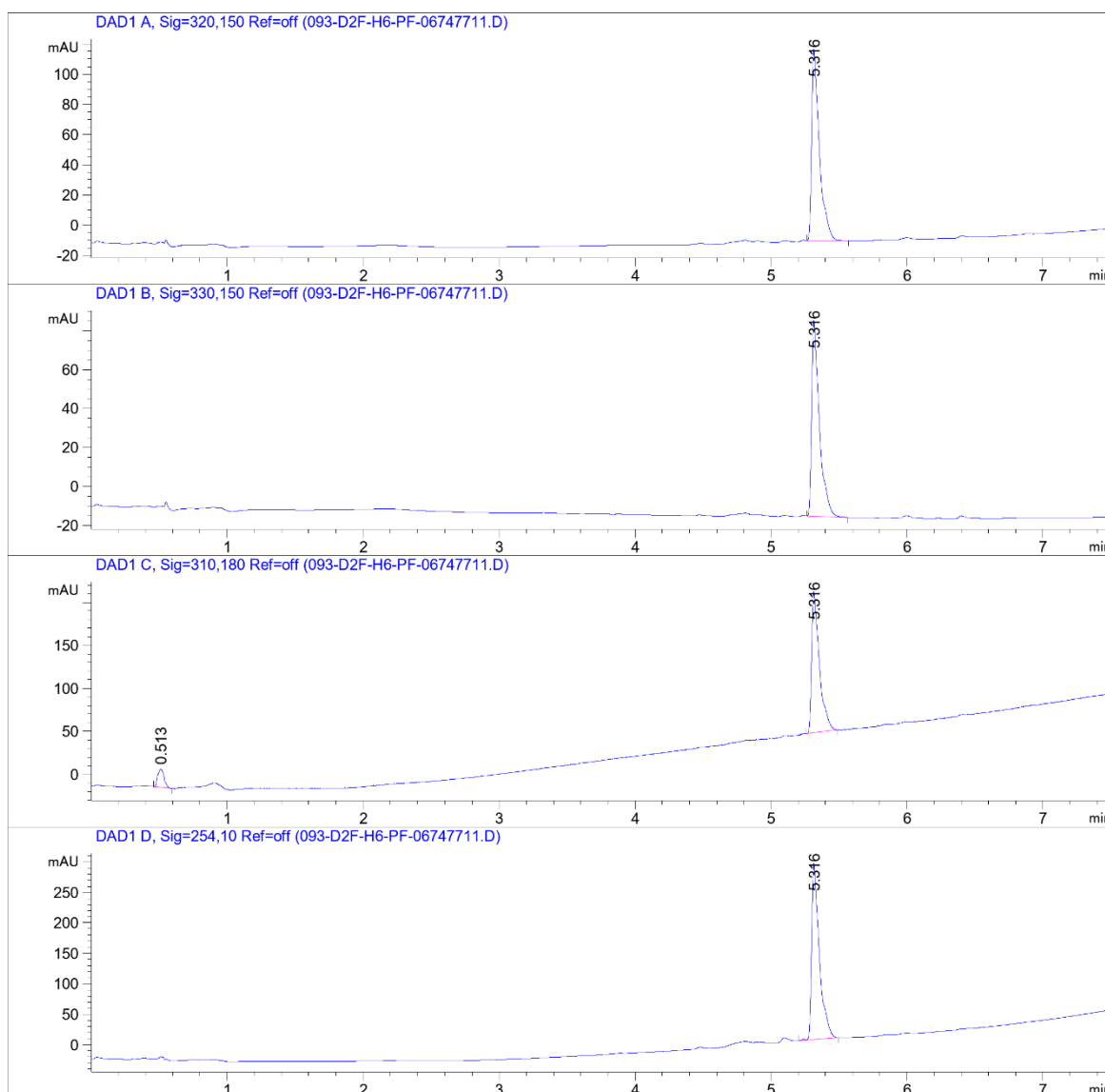
COMPOUND INFORMATION

Purity

Data File W:\analyti...\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\093-D2F-H6-PF-06747711.D

Sample Name: PF-06747711

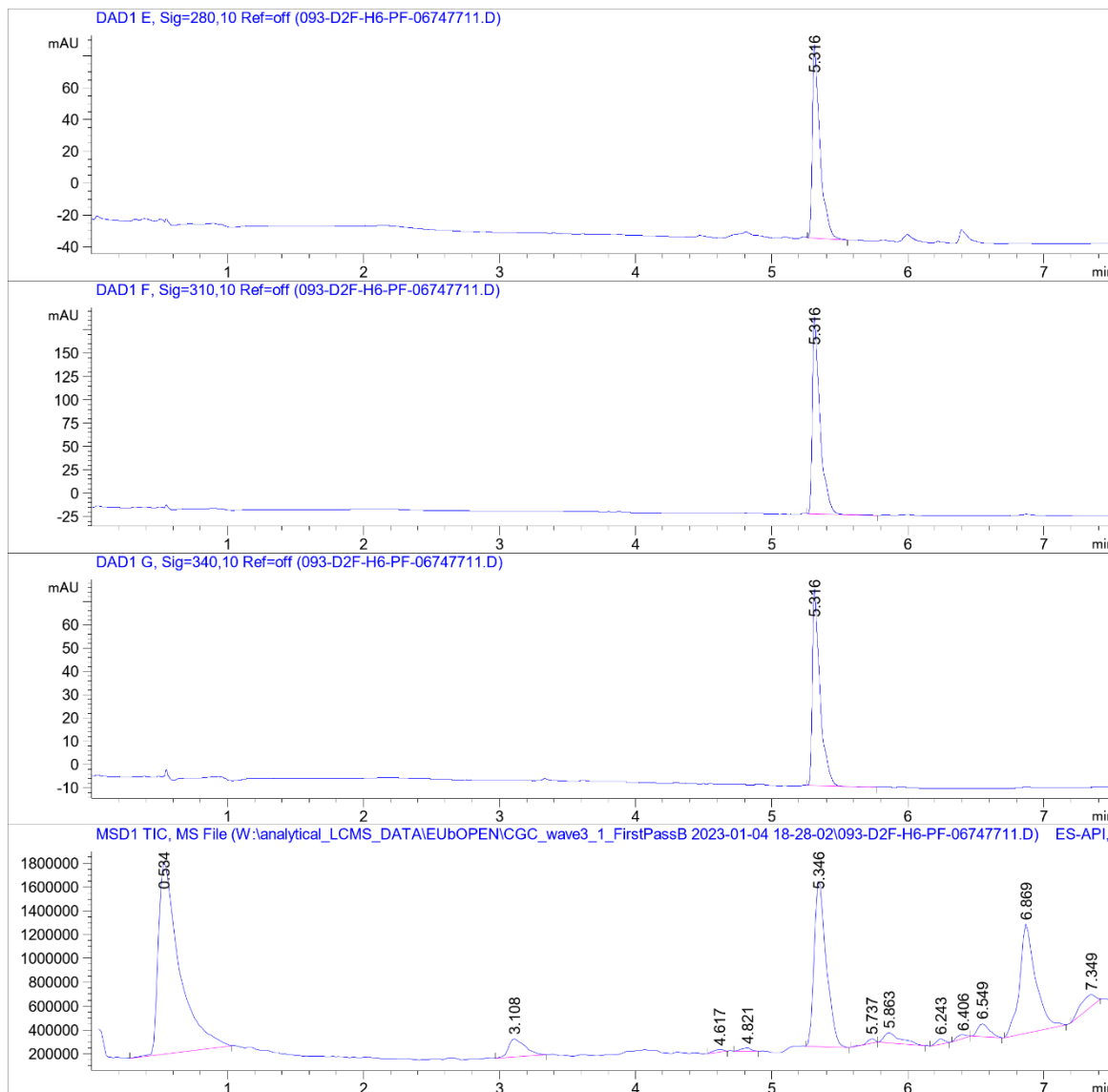
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=====
Acq. Operator   : SYSTEM                      Seq. Line :   93
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2F-H6
Injection Date  : 1/5/2023 11:28:13 AM       Inj       :    1
                                           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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Data File W:\analyti...CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\093-D2F-H6-PF-06747711.D

Sample Name: PF-06747711



COMPOUND INFORMATION

Data File W:\analyti...CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\093-D2F-H6-PF-06747711.D

Sample Name: PF-06747711

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	17254568	157.00 I
-	-	3.108	1309271	239.00 I 217.10 I
-	-	4.617	104959	170.80 I 158.20 I 137.20 I
-	-	4.821	148624	510.40 I 279.10 I 170.80 I 137.10 I
5.316	495	5.346	8638452	498.20 I
-	-	5.737	158727	280.20 I
-	-	5.863	709822	318.20 I 296.20 I
-	-	6.243	180327	228.20 I 137.10 I
-	-	6.406	162484	282.30 I 254.20 I
-	-	6.549	646716	507.20 I 485.30 I 280.20 I
-	-	6.869	7524214	282.20 I
-	-	7.349	871242	400.30 I 282.20 I

