

COMPOUND INFORMATION

DY268

CAS Registry No.: 1609564-75-1

Formal Name: 1-(3-methoxybenzyl)-N-(4-methyl-3-(morpholinosulfonyl)phenyl)-3-(p-tolyl)-1H-pyrazole-4-carboxamide

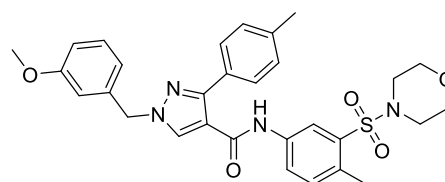
EUBOPEN ID: EUB0001174a

Molecular Formula: C₃₀H₃₂N₄O₅S

Molecular Weight: 560.67 g/mol

Smiles:
CC1=CC=C(C2=NN(C=C2C(=O)NC3=CC=C(C(S(=O)(=O)N4CCOCC4)=O)=O)C3)C=O)CC5=CC=CC(OC)=C5)C=C1

Recommended concentration: 1 μ M



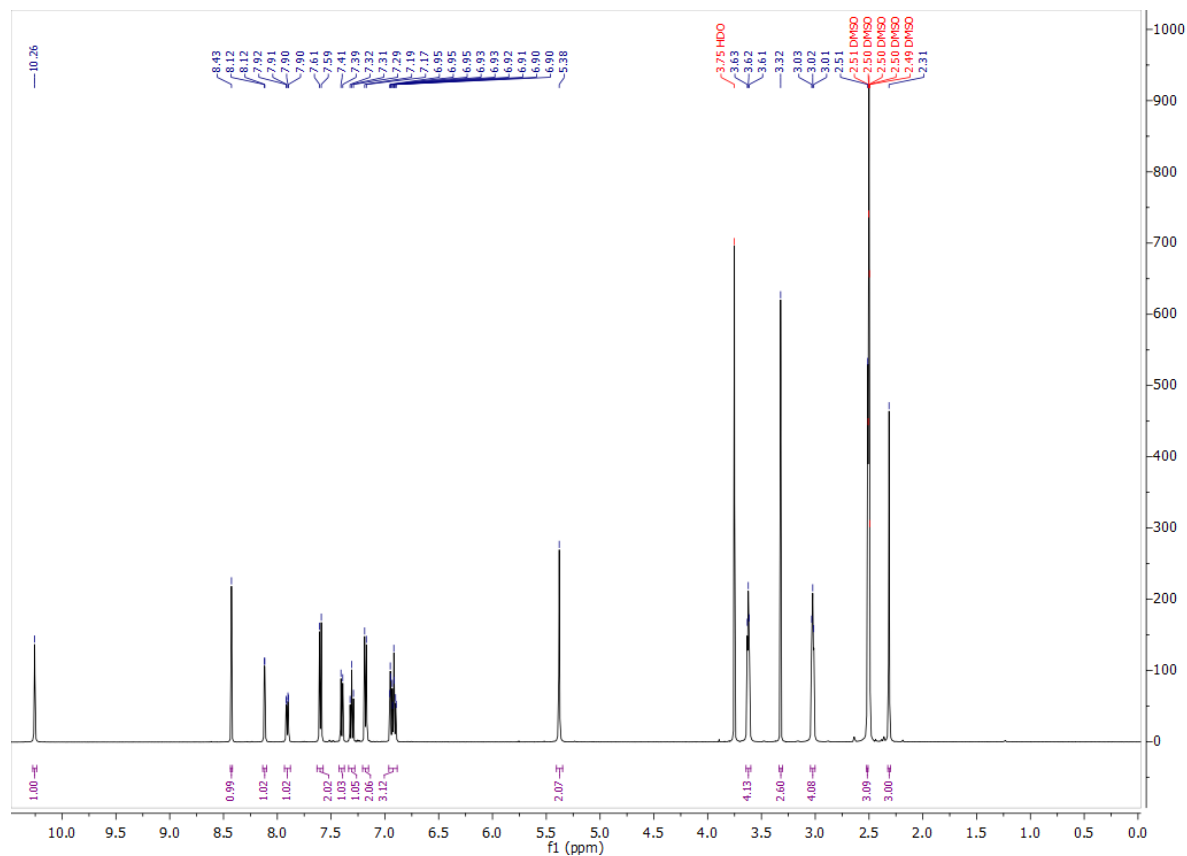
Biological activity

		Type	IC ₅₀ /EC ₅₀ [μ M]	Reference
Main NR target:	NR1H4 (FXR)	Antagonist	0.58	inhouse
NR off-target:	NR1H3 (LXR α)	Antagonist	1.6	inhouse
	NR1H2 (LXR β)	Antagonist	1.3	

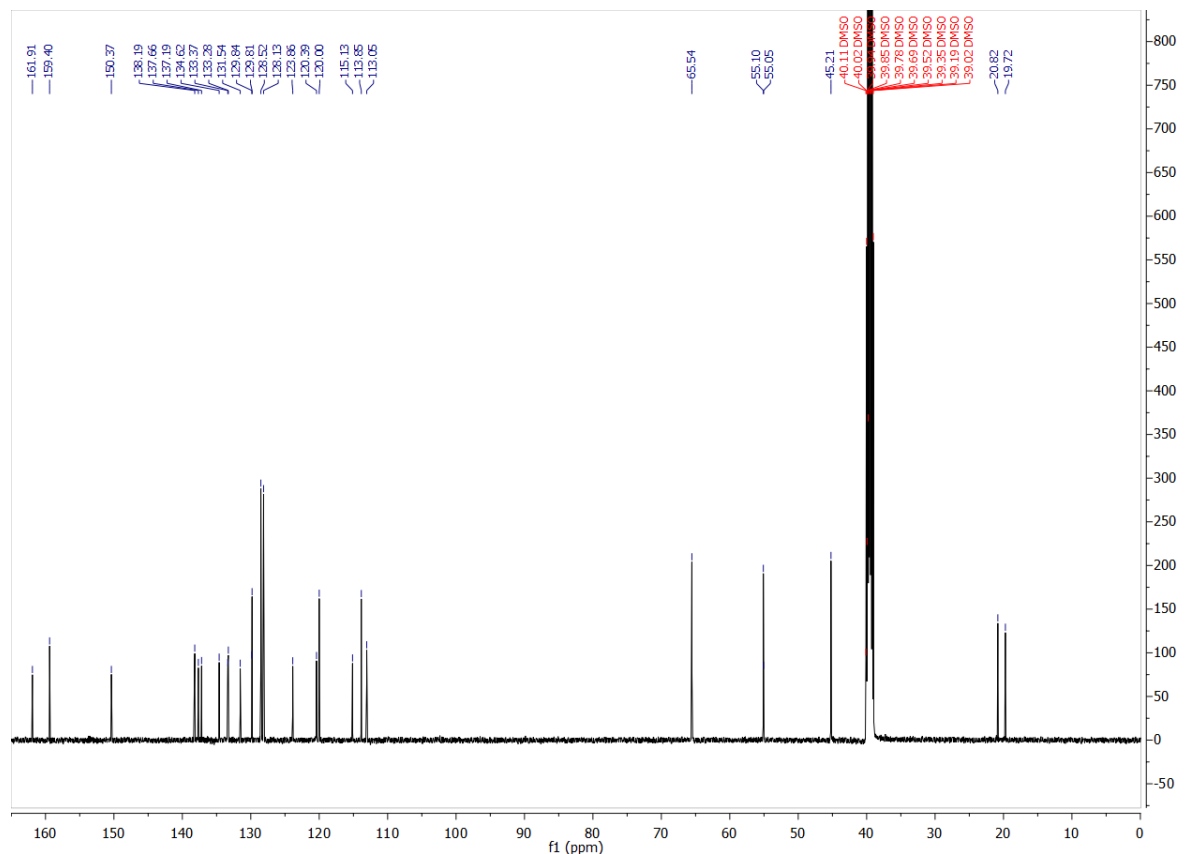
COMPOUND INFORMATION

Identity

¹H NMR



¹³C NMR



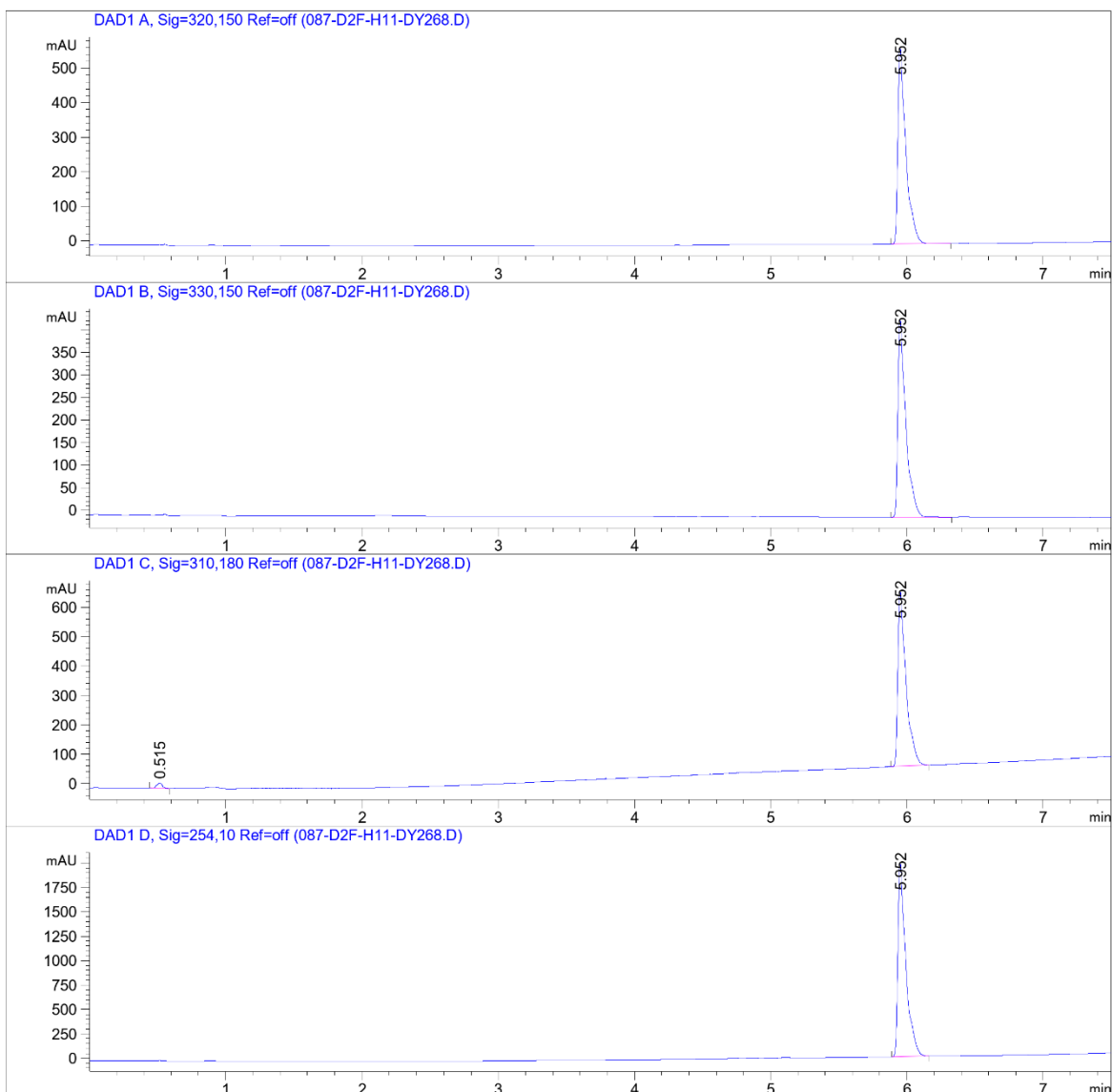
COMPOUND INFORMATION

Purity

Data File W:\analyti...OPEN\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\087-D2F-H11-DY268.D

Sample Name: DY268

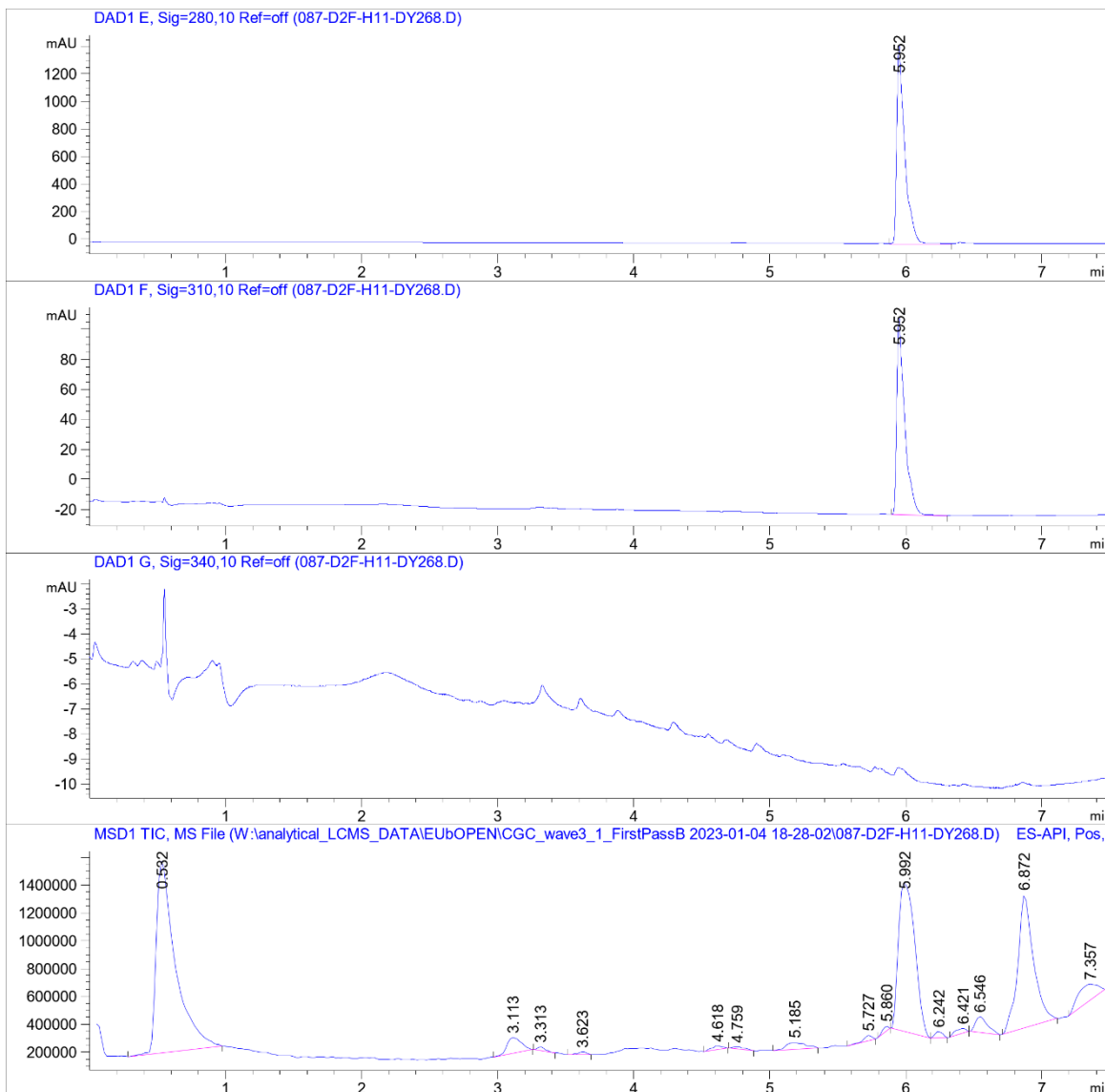
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=====
Acq. Operator   : SYSTEM                      Seq. Line :   87
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2F-H11
Injection Date  : 1/5/2023 10:21:51 AM        Inj       :    1
                                           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...OPEN\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\087-D2F-H11-DY268.D

Sample Name: DY268



COMPOUND INFORMATION



Data File W:\analyti...OPEN\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\087-D2F-H11-DY268.D

Sample Name: DY268

MS Signal: MSD1 TIC, MS File, ES-API, Pos, Scan, Frag: 70, "POS Scan"

Spectra from peak tops.

Noise Cutoff: 1000 counts.

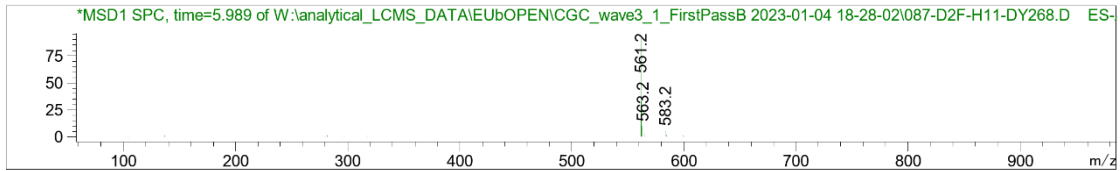
Reportable Ion Abundance: > 50%.

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
-	-	0.532	13487662	157.10 I
-	-	3.113	821931	239.00 I 217.10 I
-	-	3.313	102802	257.10 I
-	-	3.623	86049	199.90 I 170.80 I 159.00 I 137.10 I 111.10 I
-	-	4.618	149395	510.30 I 170.90 I 158.20 I 137.10 I
-	-	4.759	104362	510.40 I 279.00 I 170.90 I 137.10 I
-	-	5.185	496536	510.40 I 338.20 I 316.20 I 298.20 I 170.90 I 137.10 I 105.10 I
-	-	5.727	161107	280.20 I
-	-	5.860	107521	318.20 I 296.20 I
5.952	2288	5.992	8951491	561.20 I
-	-	6.242	180650	228.10 I 137.10 I
-	-	6.421	209454	350.20 I 282.30 I 254.20 I 137.10 I
-	-	6.546	711251	507.20 I 485.30 I 280.20 I
-	-	6.872	7675830	282.20 I
-	-	7.357	1253355	400.30 I 282.20 I

COMPOUND INFORMATION



Biological activity

