

Fexaramine

CAS Registry No.: 574013-66-4

Formal Name: Methyl (E)-3-(3-(N-((4-(dimethylamino)-[1,1'-biphenyl]-4-yl)methyl)cyclohexanecarboxamido)phenyl)acrylate

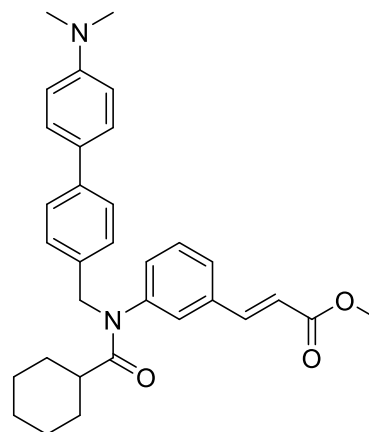
EUBOPEN ID: EUB0000182b

Molecular Formula: C₃₂H₃₆N₂O₃

Molecular Weight: 496.65 g/mol

Smiles: CN(C1=CC=C(C2=CC=C(CN(C(C3CCCC3)=O)C4=CC=CC(/C=C/C(OC)=O)=C4)C=C2)C=C1)C

Recommended concentration: 1 μM

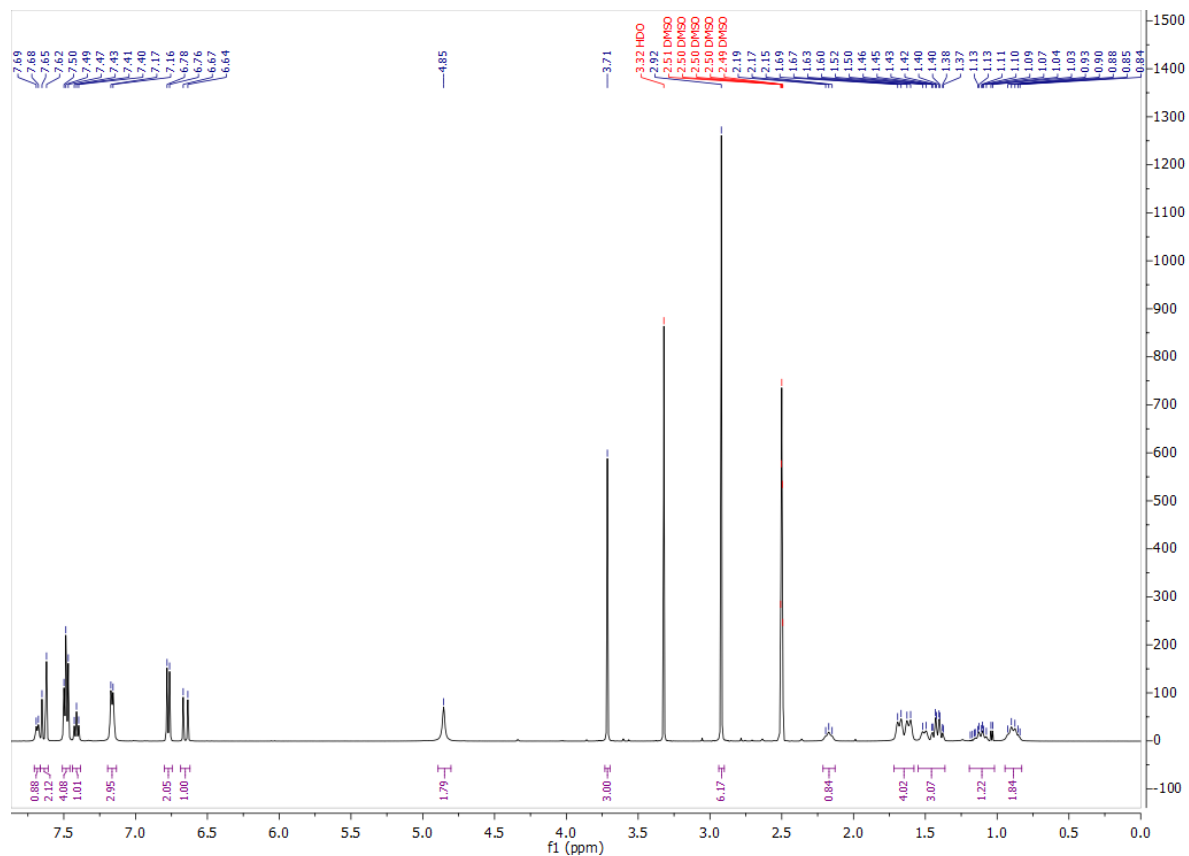


Biological activity

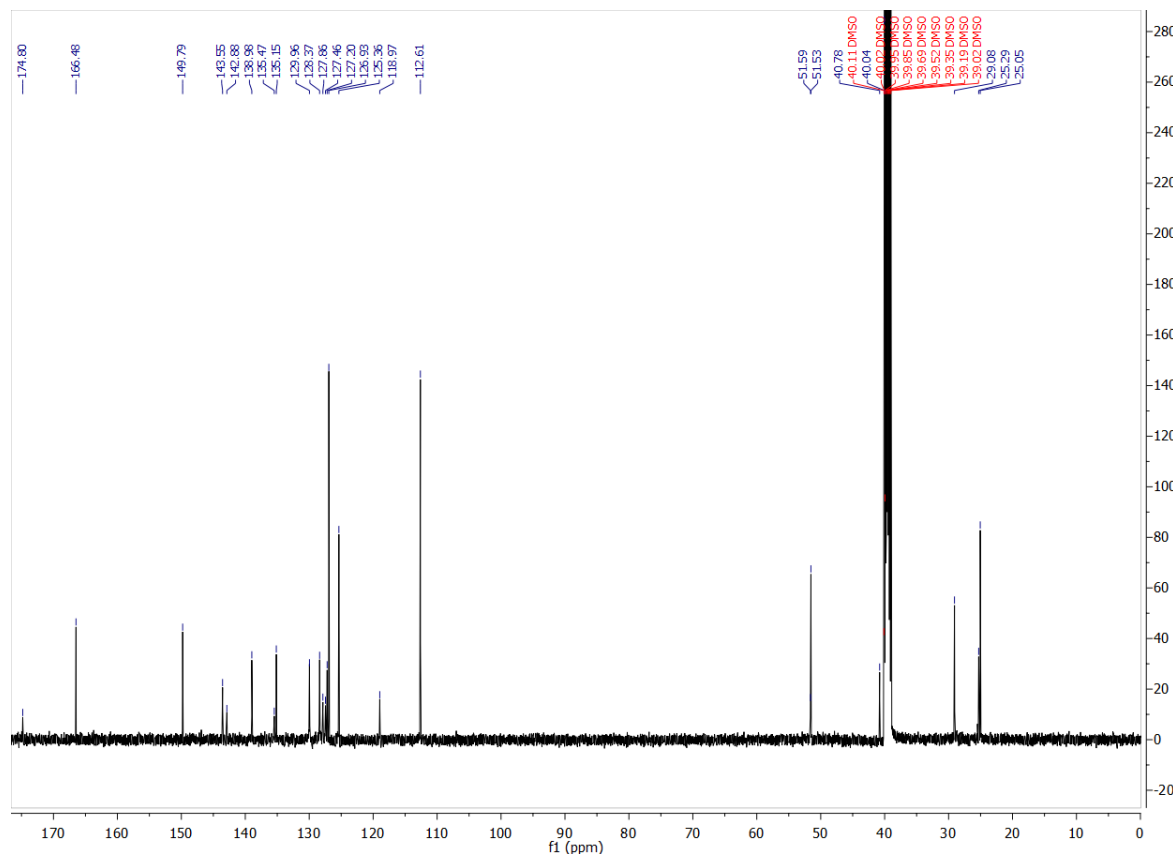
		Type	IC ₅₀ /EC ₅₀ [μM]	Reference
Main NR target:	NR1H4 (FXR)	Agonist	0.96	inhouse
NR off-target:				

Identity

¹H NMR



¹³C NMR



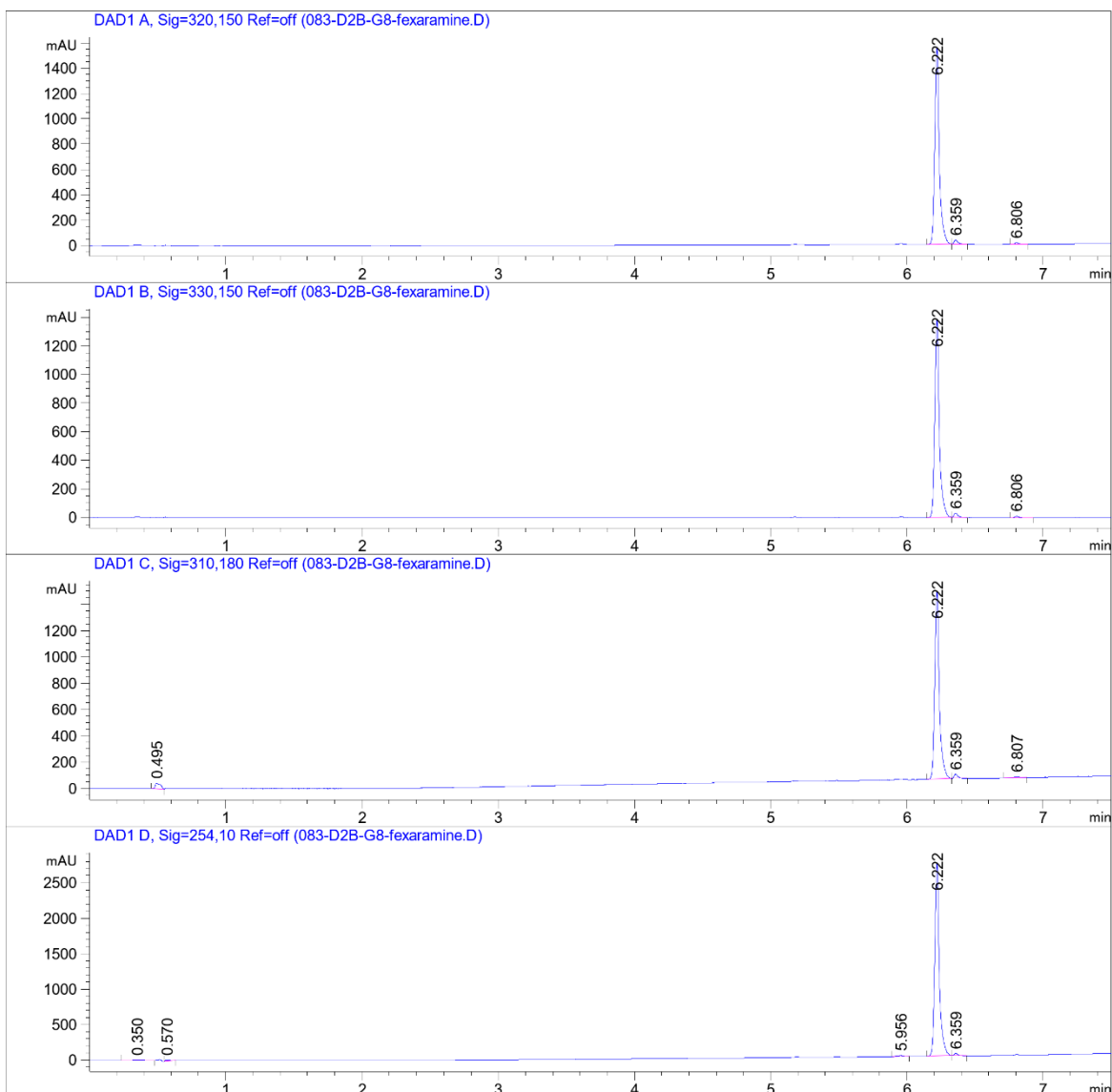
COMPOUND INFORMATION

Purity

Data File W:\analyti...\N\CGC_ECH01-3_FirstPass 2021-03-20 13-21-54\083-D2B-G8-fexaramine.D

Sample Name: fexaramine

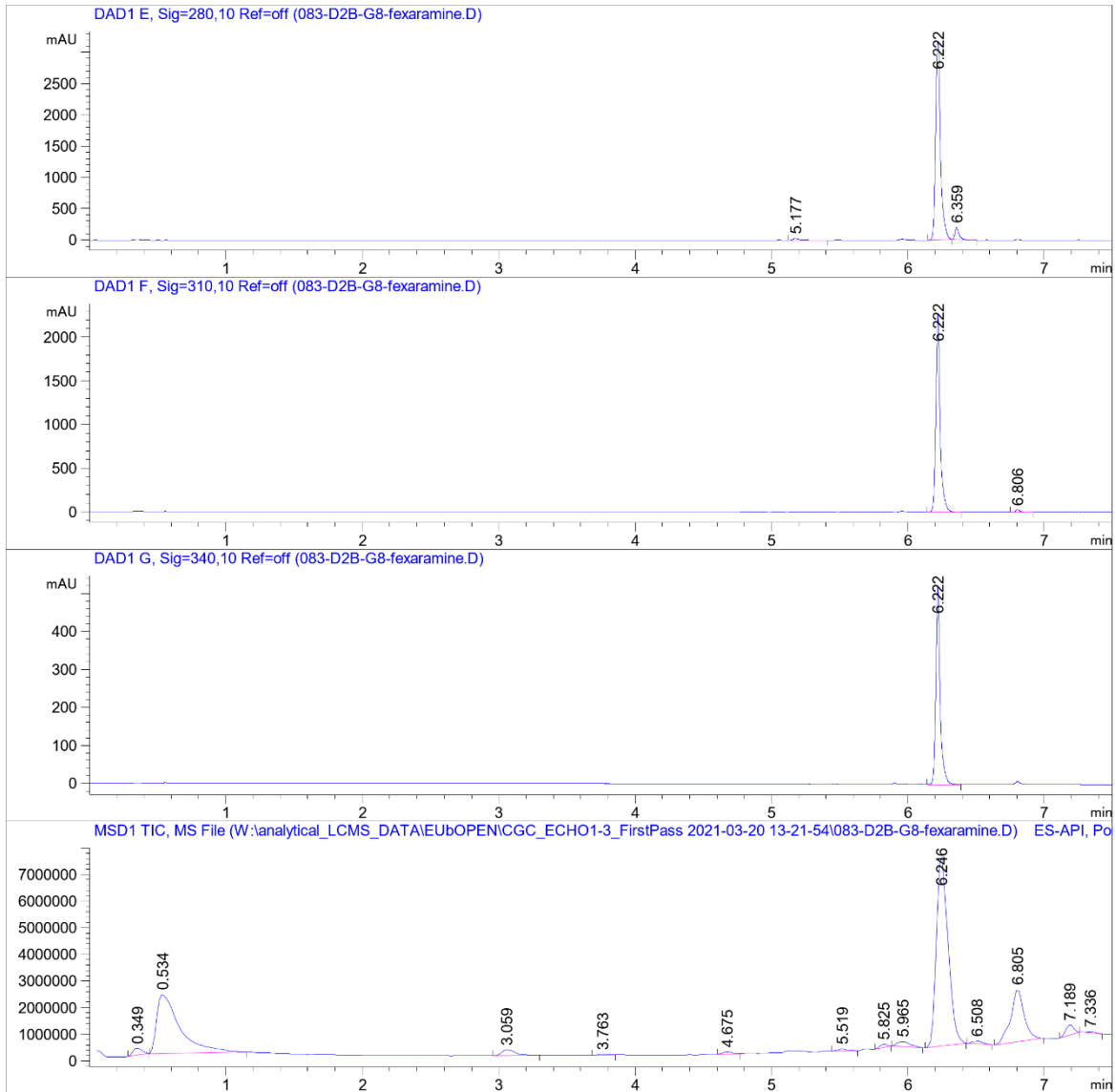
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=====
Acq. Operator   : SYSTEM                      Seq. Line :   83
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2B-G8
Injection Date  : 3/21/2021 4:34:23 AM       Inj       :    1
                                           Inj Volume: Inj prog
Sequence File   : W:\analytical_LCMS_DATA\EUBOPEN\CGC_ECH01-3_FirstPass 2021-03-20 13-21-54
                  \CGC_ECH01-3_FirstPass.S
Method          : W:\analytical_LCMS_DATA\EUBOPEN\CGC_ECH01-3_FirstPass 2021-03-20 13-21-54
                  \CGL_FIRSTPASS_GENERALMETHOD_VIAL3+4_20210319.M (Sequence Method)
Last changed    : 3/19/2021 5:35:24 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_ECH01-3_FirstPass 2021-03-20 13-21-54\083-D2B-G8-fexaramine.D

Sample Name: fexaramine



COMPOUND INFORMATION

Data File W:\analyti...\CGC_ECHO1-3_FirstPass 2021-03-20 13-21-54\083-D2B-G8-fexaramine.D

Sample Name: fexaramine

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

Spectra from peak tops.

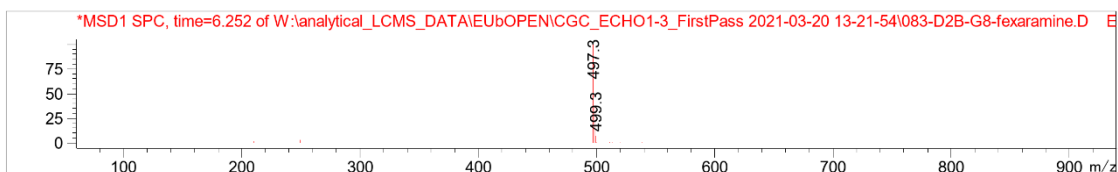
Noise Cutoff: 1000 counts.

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
-	-	0.349	1175882	182.90 I 158.00 I
-	-	0.534	26096508	157.00 I
-	-	3.059	1444823	217.10 I
-	-	3.763	181934	274.20 I
-	-	4.675	412686	326.30 I
-	-	5.519	379627	469.20 I
-	-	5.825	494745	296.20 I
-	-	5.965	1336074	483.30 I
6.222	3603	6.246	42136496	497.30 I
6.359	61	-	-	
-	-	6.508	583749	485.30 I 280.20 I
6.806	26	6.805	13365873	282.20 I
-	-	7.189	1514970	284.30 I 282.20 I
-	-	7.336	232825	400.30 I 282.20 I



COMPOUND INFORMATION

Biological activity

Fexaramine
FXR - EC₅₀ 0.96 ± 0.05 μM
60 ± 2 fold activation

