

# COMPOUND INFORMATION

## XL335

**CAS Registry No.:** 629664-81-9

**Formal Name:** Isopropyl 3-(3,4-difluorobenzoyl)-1,1-dimethyl-1,2,3,6-tetrahydroazepino[4,5-b]indole-5-carboxylate

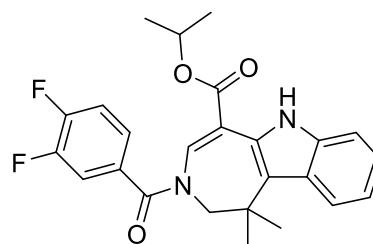
**EUBOPEN ID:** EUB0000573a

**Molecular Formula:** C<sub>25</sub>H<sub>24</sub>F<sub>2</sub>N<sub>2</sub>O<sub>3</sub>

**Molecular Weight:** 438.47 g/mol

**Smiles:** CC(OC(C1=CN(C(C2=CC(F)=C(F)C=C2)=O)CC(C)(C)C3=C1NC4=CC=CC=C43)=O)C

**Recommended concentration:** 1  $\mu$ M



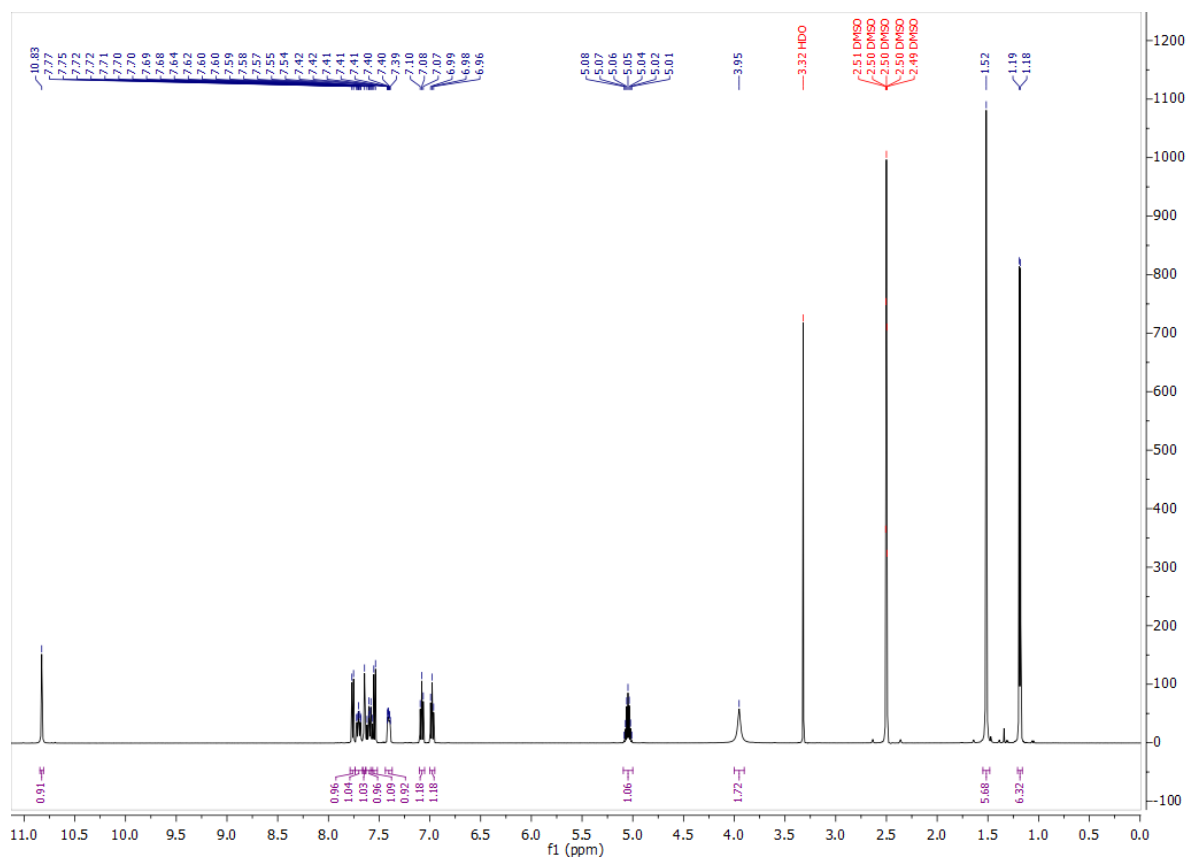
### Biological activity

		Type	IC <sub>50</sub> /EC <sub>50</sub> [ $\mu$ M]	Reference
Main NR target:	NR1H4 (FXR)	Agonist	0.099	inhouse
NR off-target:				

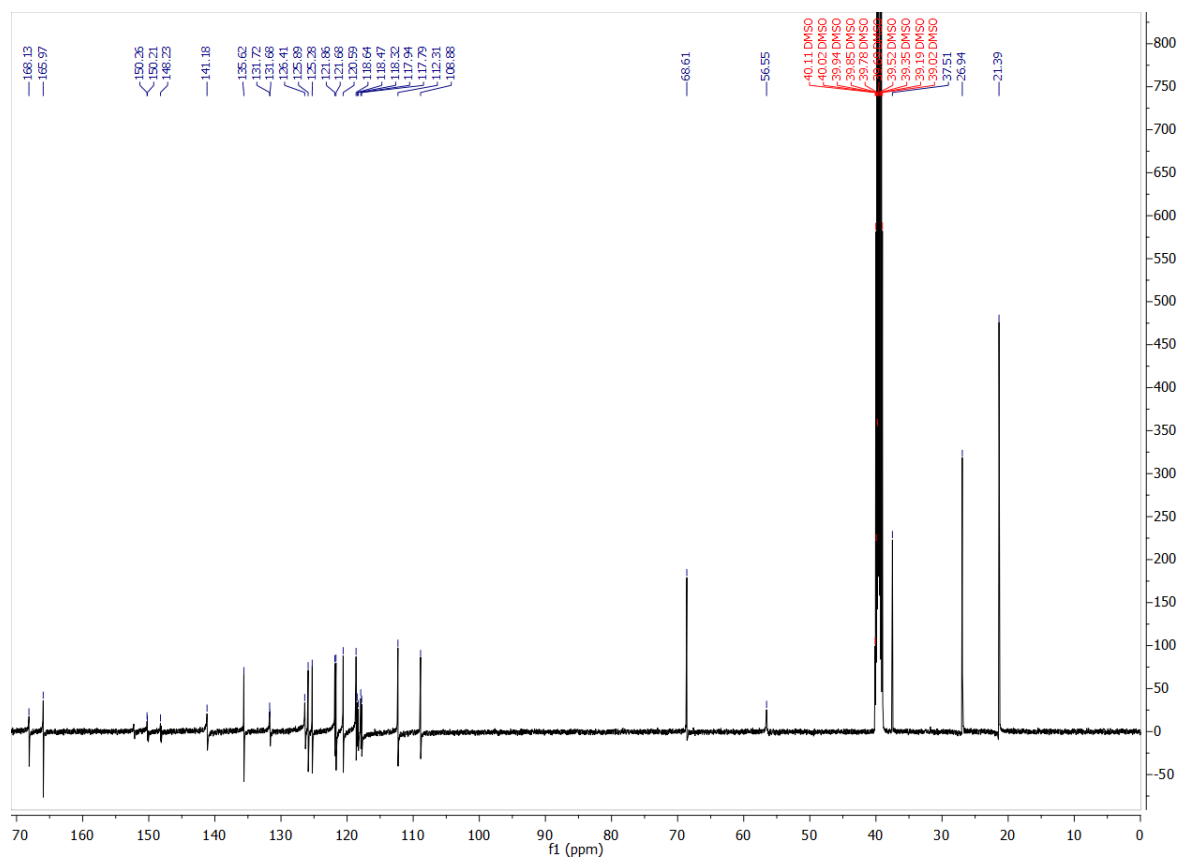
# COMPOUND INFORMATION

## Identity

### <sup>1</sup>H NMR



### <sup>13</sup>C NMR



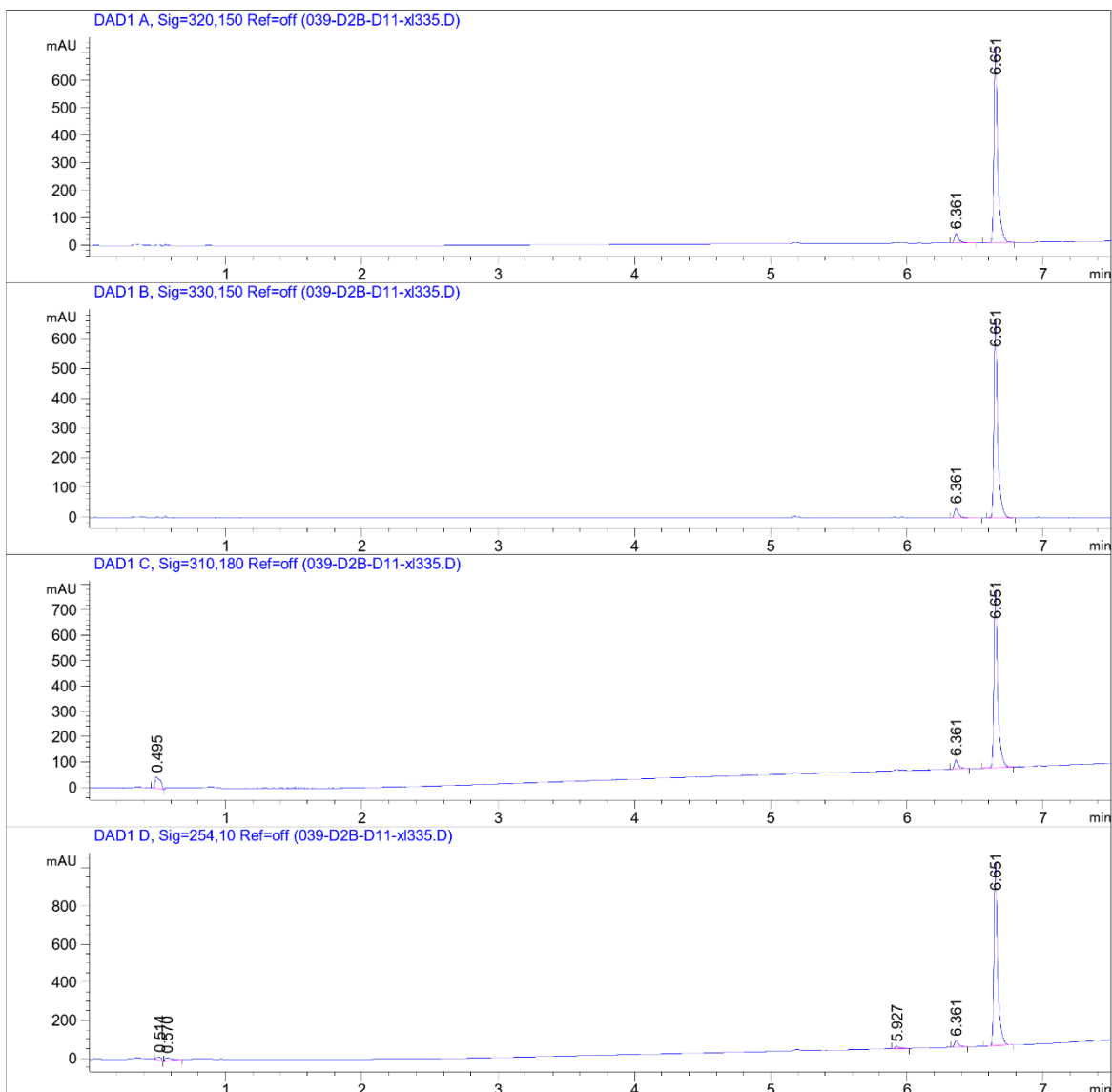
# COMPOUND INFORMATION

## Purity

Data File W:\analyti...bOPEN\CGC\_ECH01-3\_FirstPass 2021-03-20 13-21-54\039-D2B-D11-x1335.D

Sample Name: x1335

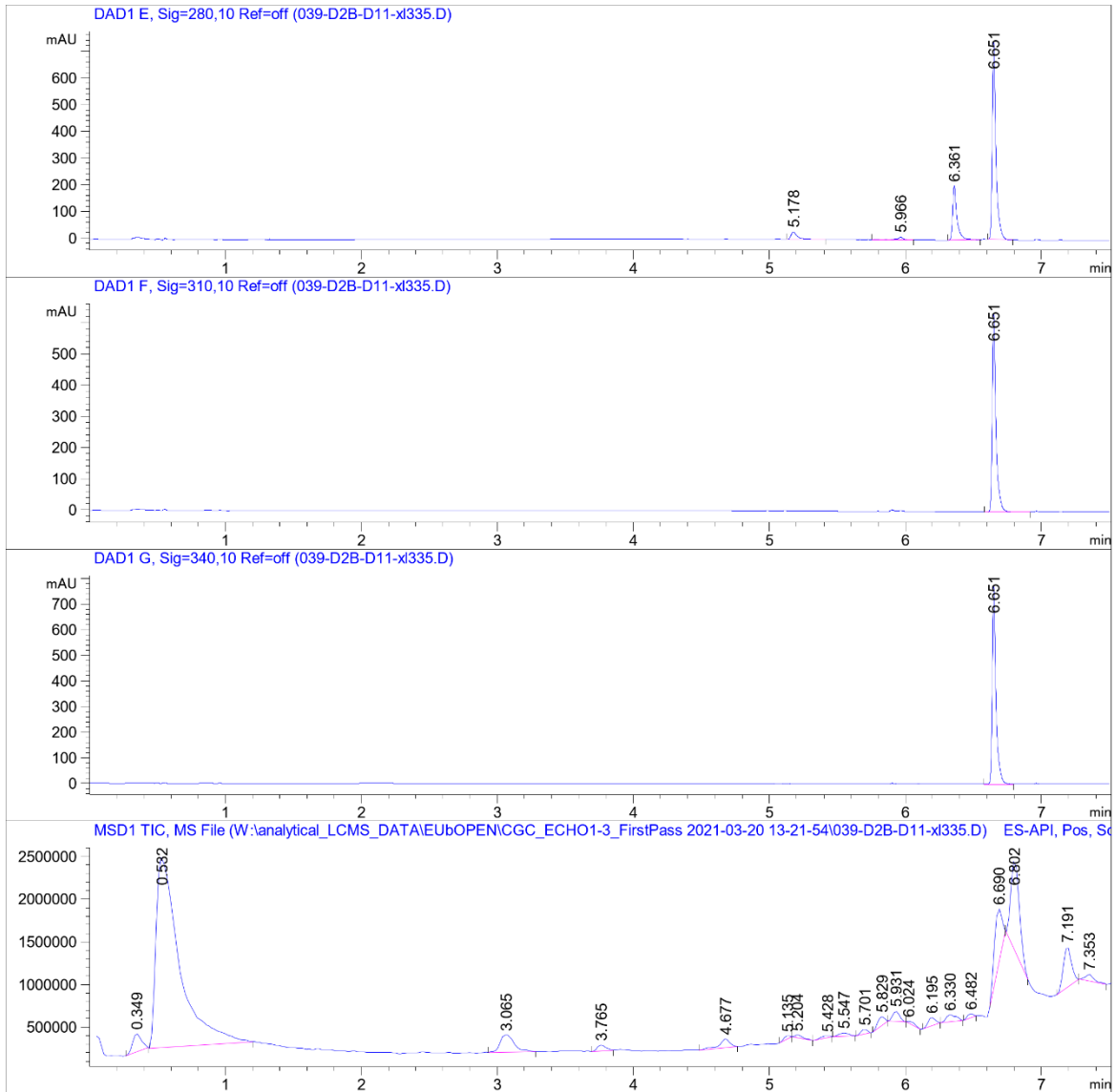
```
=====
Acq. Operator   : SYSTEM                      Seq. Line :   39
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2B-D11
Injection Date  : 3/20/2021 8:26:46 PM       Inj       :    1
                                           Inj Volume: Inj prog
Sequence File   : 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
=====
```



# COMPOUND INFORMATION

Data File W:\analyti...bOPEN\CGC\_ECHO1-3\_FirstPass 2021-03-20 13-21-54\039-D2B-D11-x1335.D

Sample Name: x1335



# COMPOUND INFORMATION



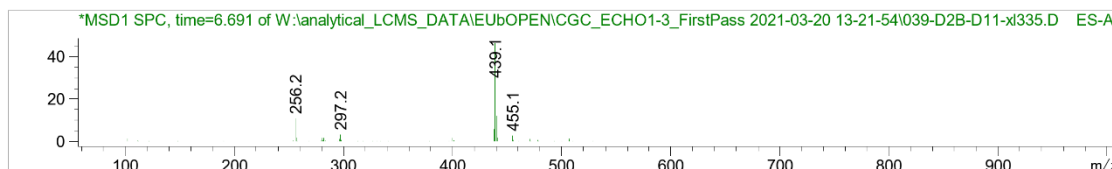
Data File W:\analyti...bOPEN\CGC\_ECH01-3\_FirstPass 2021-03-20 13-21-54\039-D2B-D11-x1335.D

Sample Name: x1335

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	975039	158.00 I 130.00 I
-	-	0.532	26800514	157.00 I
-	-	3.065	1428043	217.00 I
-	-	3.765	289226	274.20 I
-	-	4.677	549076	326.40 I
-	-	5.135	98579	298.20 I 295.10 I 225.10 I 102.10 I
-	-	5.204	126551	316.20 I 111.00 I 102.10 I
-	-	5.428	100580	310.20 I 111.10 I 102.10 I
-	-	5.547	208128	326.20 I 282.20 I 280.20 I 102.10 I
-	-	5.701	172443	280.20 I
-	-	5.829	362638	296.20 I
-	-	5.931	418153	296.20 I 280.20 I
-	-	6.024	111913	298.20 I 296.30 I 280.20 I 102.20 I
-	-	6.195	360092	280.20 I 228.20 I
6.361	73	6.330	428097	254.20 I
-	-	6.482	144000	280.20 I
6.651	1333	6.690	2542721	439.10 I
-	-	6.802	4482313	282.20 I
-	-	7.191	1959236	284.20 I 282.20 I
-	-	7.353	344395	400.30 I 282.20 I

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## Biological activity

**XL335**  
FXR - EC<sub>50</sub> 0.099 ± 0.009 μM  
315 ± 7 fold activation

