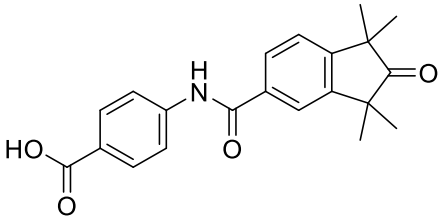
COMPOUND INFORMATION

BMS753

CAS Registry No.:	215307-86-1
Formal Name:	4-(1,1,3,3-tetramethyl-2-oxo-2,3-dihydro-1H-indene-5-carboxamido)benzoic acid
EUbOPEN ID:	EUB0000565a
Molecular Formula:	$C_{21}H_{21}NO_4$
Molecular Weight:	351.40 g/mol
Smiles:	CC1(C2=C(C=C(C=C2)C(=O)NC3=CC=C(C=C3)C(=O)O)C(C1=O)(C)C)C
Recommended concentration:	1 µM



Biological activity

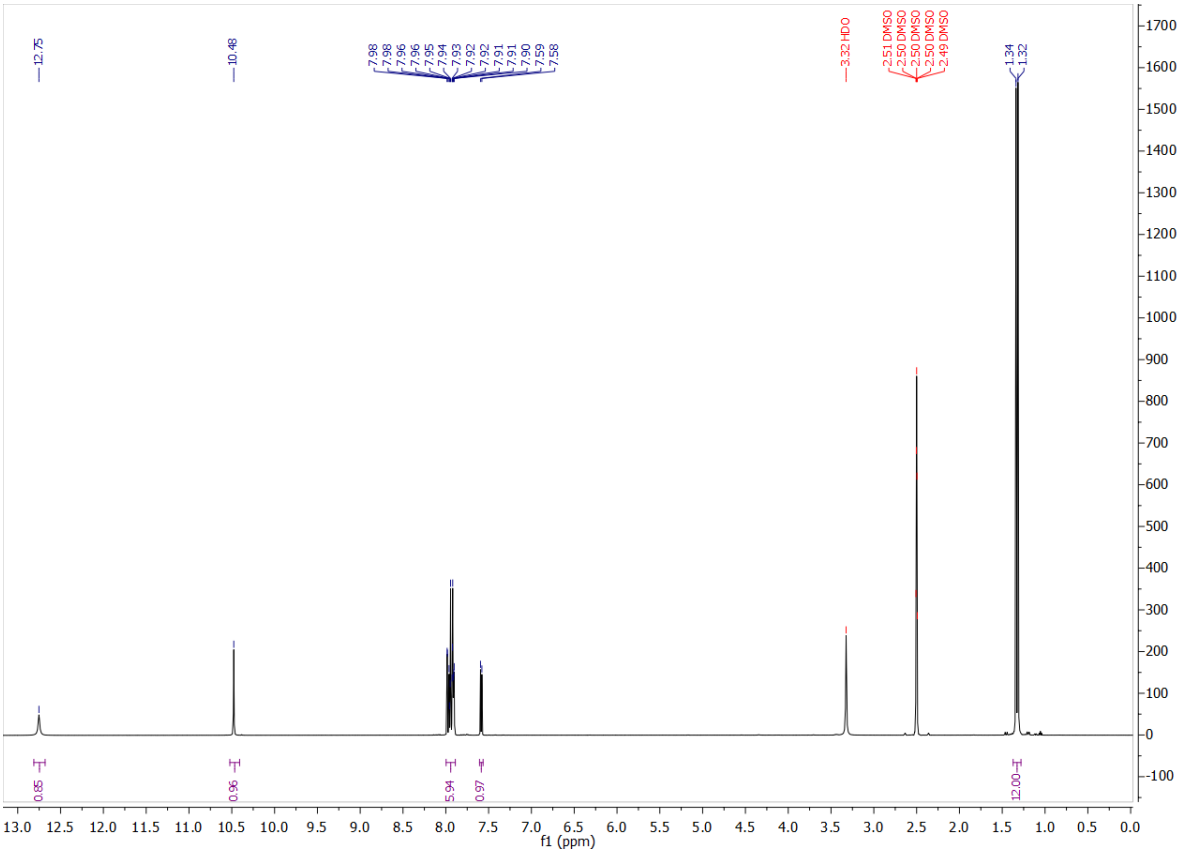
		Type	IC_{50}/EC_{50} [µM]	Reference
Main target:	NR1B1 (RARα)	Agonist	0.11	inhouse

Off-targets:

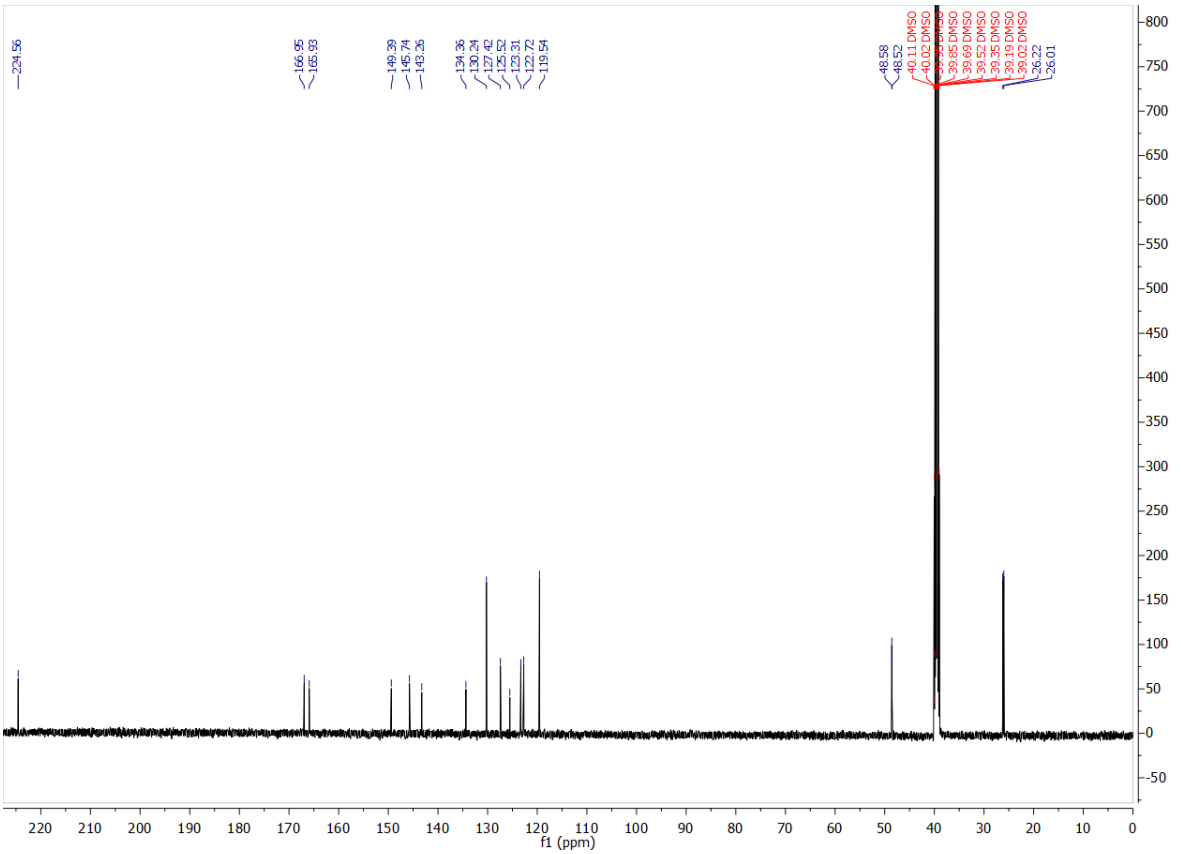
COMPOUND INFORMATION

Identity

^{1}H NMR



^{13}C NMR



COMPOUND INFORMATION

Purity

Data File W:\analyti...OPEN\CGC_ECHO1-3_FirstPass 2021-03-20 13-21-54\004-D2B-A12-BMS753.D
Sample Name: BMS753

```
======================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   4
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                      Location :   D2B-A12
Injection Date  : 3/20/2021 1:58:50 PM               Inj :   1
                                                Inj Volume : Inj prog
Sequence File   : W:\analytical_LCMS_DATA\EUbOPEN\CGC_ECHO1-3_FirstPass 2021-03-20 13-21-54
                  \CGC_ECHO1-3_FirstPass.S
Method          : W:\analytical_LCMS_DATA\EUbOPEN\CGC_ECHO1-3_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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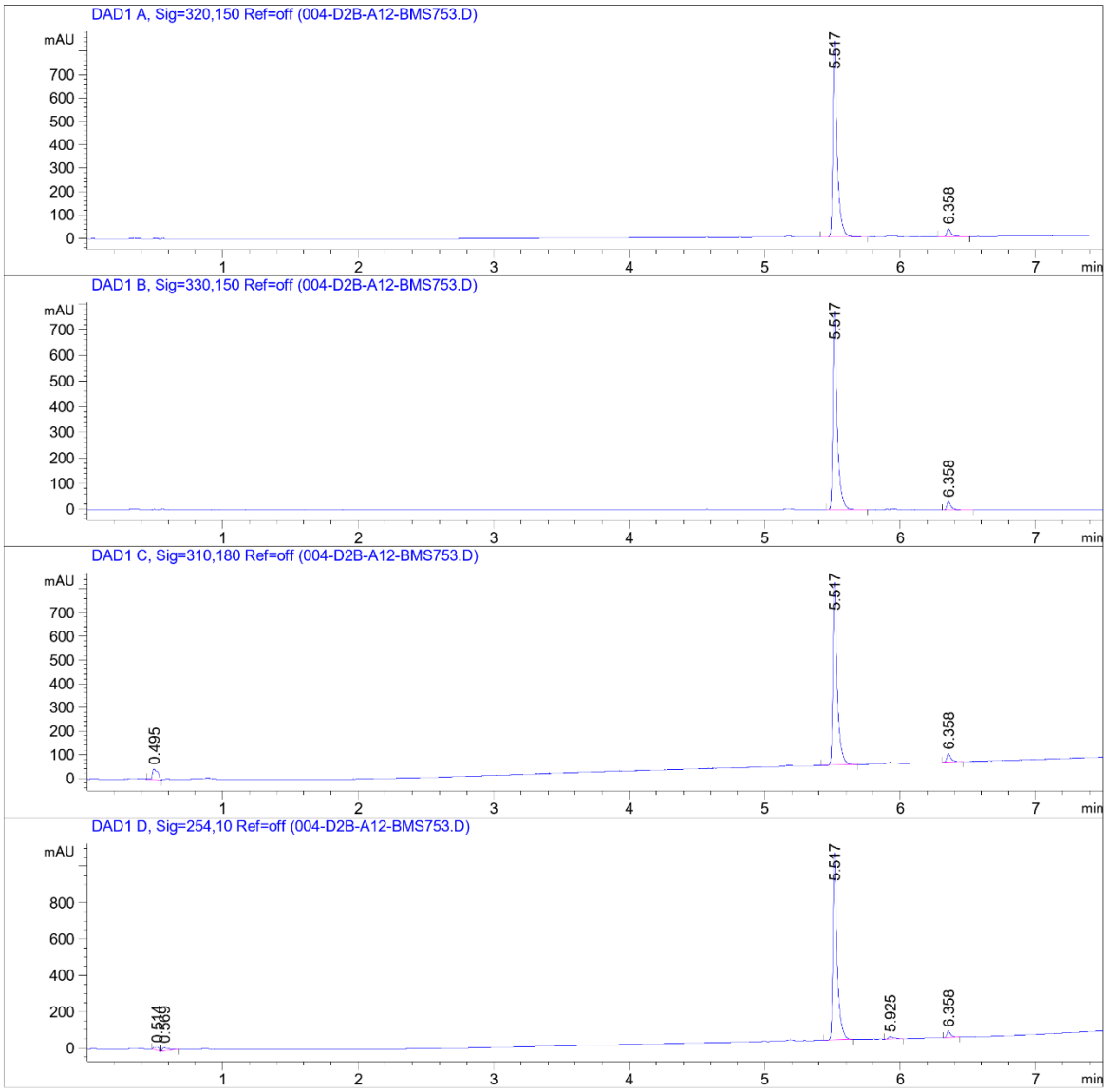
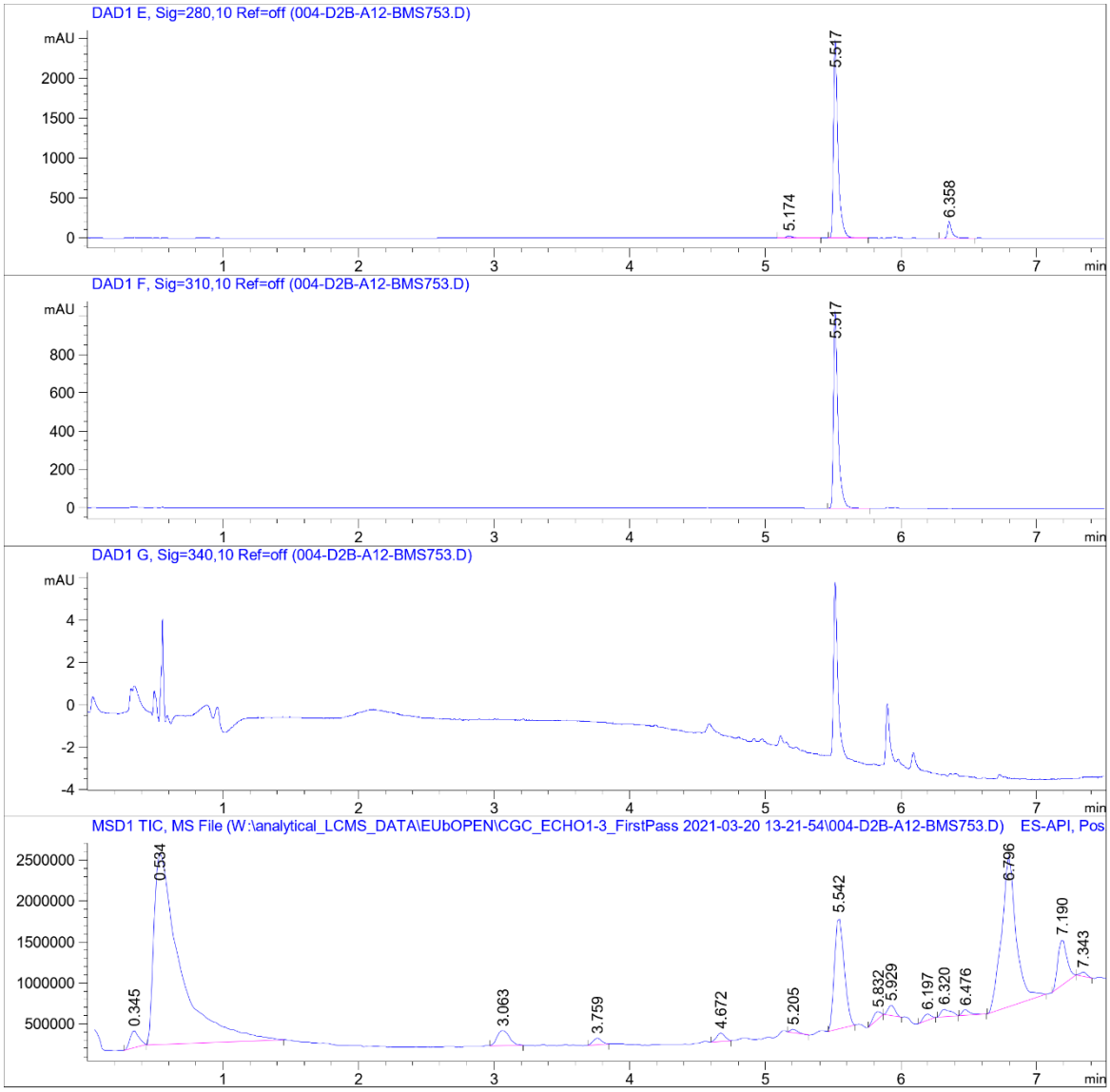


COMPOUND INFORMATION

Data File W:\analyti...OPEN\CGC_ECHO1-3_FirstPass 2021-03-20 13-21-54\004-D2B-A12-BMS753.D
Sample Name: BMS753

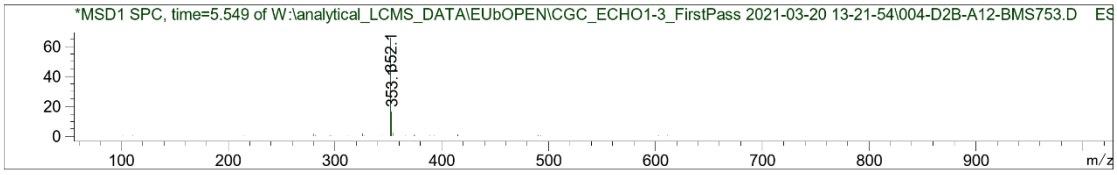


COMPOUND INFORMATION

Data File W:\analyti...OPEN\CGC_ECHO1-3_FirstPass 2021-03-20 13-21-54\004-D2B-A12-BMS753.D
Sample Name: BMS753

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
-	-	0.345	938060	158.00 I
-	-	0.534	31501578	157.00 I
-	-	3.063	1183681	217.10 I
-	-	3.759	363428	274.20 I
-	-	4.672	435477	326.30 I
-	-	5.205	153765	316.20 I 298.20 I 199.90 I 158.90 I 111.10 I 102.10 I
5.517	1895	5.542	6701950	352.10 I
-	-	5.832	353985	296.20 I
-	-	5.929	457770	296.20 I 294.20 I 280.30 I
-	-	6.197	303301	280.20 I 228.20 I
6.358	76	6.320	476307	254.20 I
-	-	6.476	301237	280.20 I
-	-	6.796	13585264	282.30 I
-	-	7.190	2593089	284.20 I 282.20 I
-	-	7.343	184609	400.30 I 282.20 I



COMPOUND INFORMATION

Biological activity