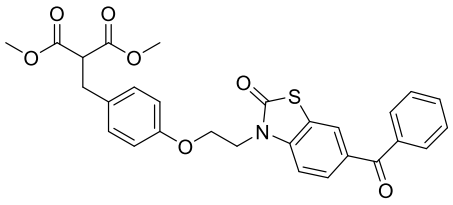
COMPOUND INFORMATION

S26948

CAS Registry No.:	353280-43-0
Formal Name:	Dimethyl 2-(4-(2-(6-benzoyl-2-oxobenzo[d]thiazol-3(2H)-yl)ethoxy)benzyl)malonate
EUbOPEN ID:	EUB0000571a
Molecular Formula:	$C_{28}H_{25}NO_7S$
Molecular Weight:	519.57 g/mol
Smiles:	COC(=O)C(CC1=CC=C(C=C1)OCCN2C3=C(C=C(C=C3)C(=O)C4=CC=CC=C4)SC2=O)C(=O)OC
Recommended concentration:	1 µM



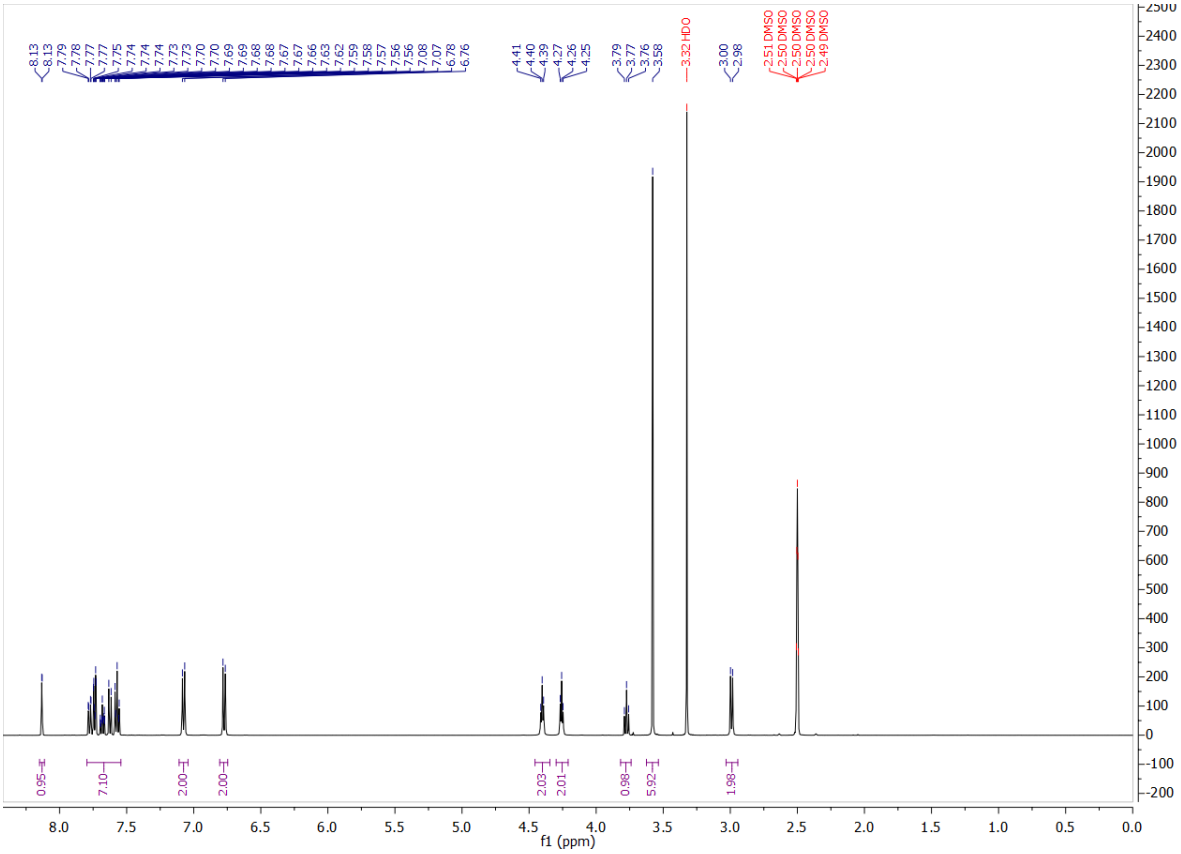
Biological activity

		Type	IC_{50}/EC_{50} [µM]	Reference
Main NR target:	NR1C3 (PPARγ)	Agonist	0.042	inhouse
NR off-target:				

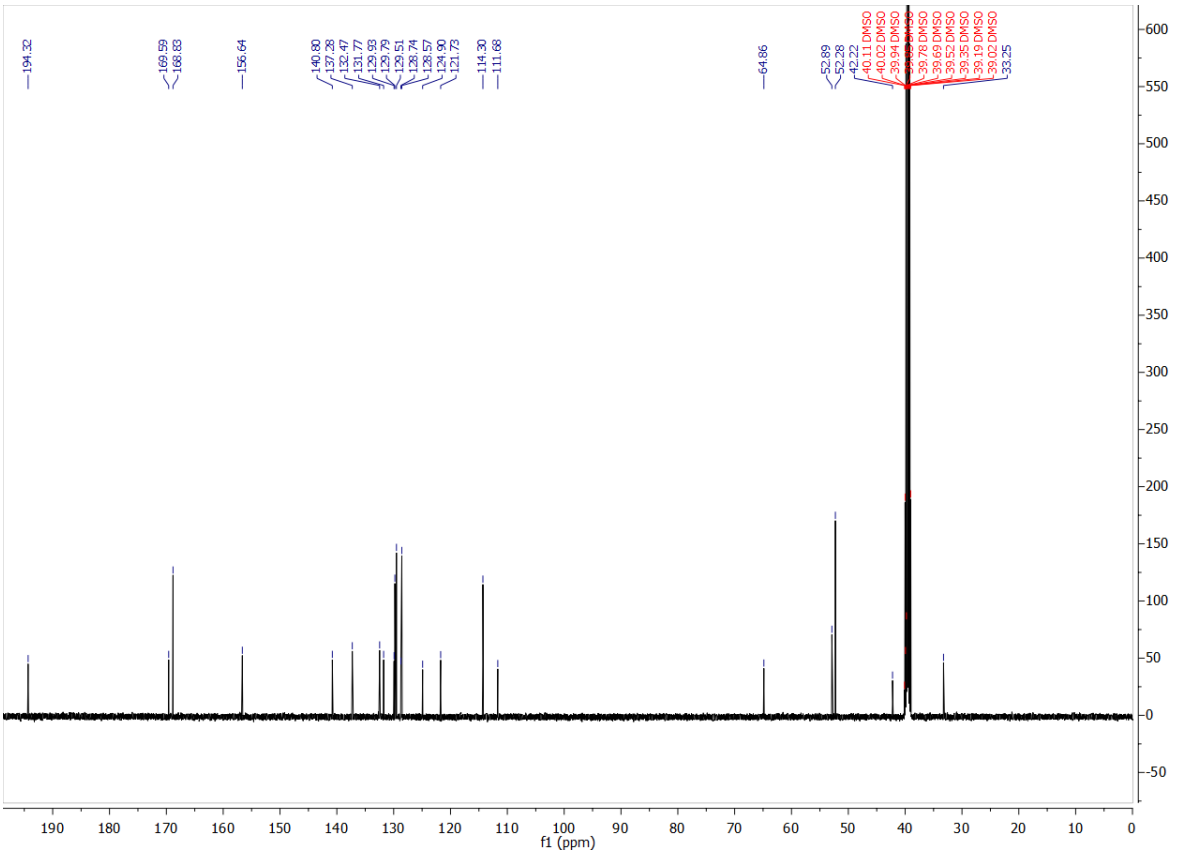
COMPOUND INFORMATION

Identity

^{1}H NMR



^{13}C NMR

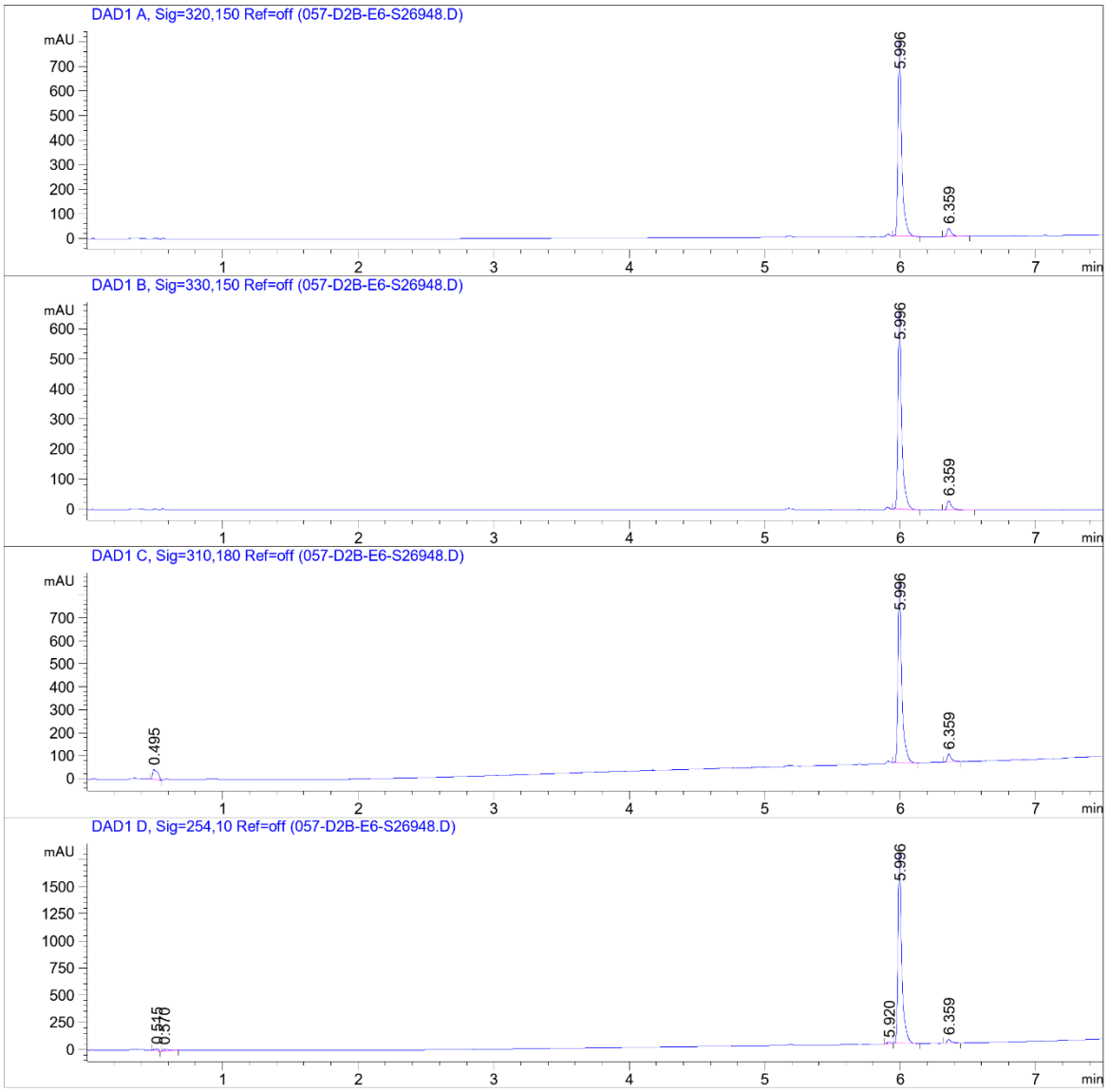


COMPOUND INFORMATION

Purity

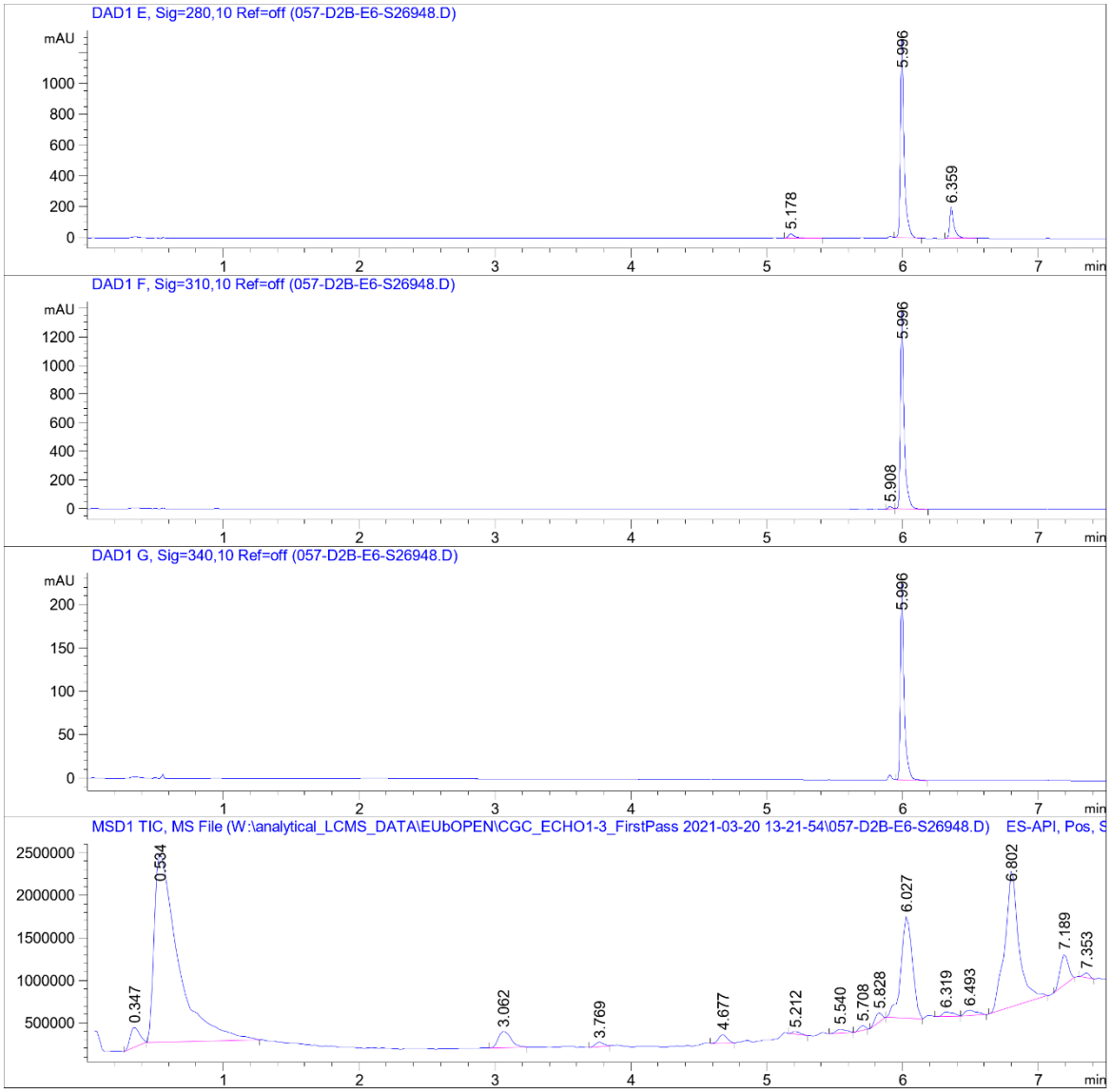
Data File W:\analyti...bOPEN\CGC_ECHO1-3_FirstPass 2021-03-20 13-21-54\057-D2B-E6-S26948.D
Sample Name: S26948

```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :  57
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                      Location :  D2B-E6
Injection Date  : 3/20/2021 11:46:12 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
```



COMPOUND INFORMATION

Data File W:\analyti...bOPEN\CGC_ECHO1-3_FirstPass 2021-03-20 13-21-54\057-D2B-E6-S26948.D
Sample Name: S26948

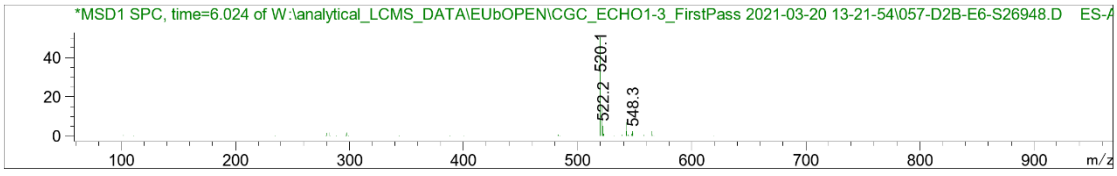


COMPOUND INFORMATION

Data File W:\analyti...bOPEN\CGC_ECHO1-3_FirstPass 2021-03-20 13-21-54\057-D2B-E6-S26948.D
Sample Name: S26948

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
-	-	0.347	1083867	158.00 I
-	-	0.534	27272738	157.00 I
-	-	3.062	1219014	217.00 I
-	-	3.769	229397	274.20 I
-	-	4.677	447964	326.30 I
-	-	5.212	120461	316.20 I 102.10 I
-	-	5.540	237806	326.20 I 295.10 I 282.20 I 280.20 I 102.20 I
-	-	5.708	171409	280.20 I
-	-	5.828	395846	296.20 I
5.996	1514	6.027	7025183	520.10 I
6.359	74	6.319	304671	254.20 I
-	-	6.493	372301	280.20 I
-	-	6.802	11450855	282.20 I
-	-	7.189	1519516	284.30 I 282.20 I
-	-	7.353	156871	400.30 I 282.20 I



COMPOUND INFORMATION

Biological activity