

## Tazarotene

**CAS Registry No.:** 118292-40-3

**Formal Name:** Ethyl 6-((4,4-dimethylthiochroman-6-yl)ethynyl)nicotinate

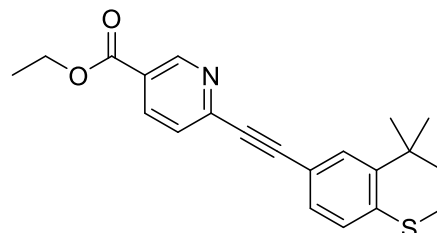
**EUbOPEN ID:** EUB0000563a

**Molecular Formula:** C<sub>21</sub>H<sub>21</sub>NO<sub>2</sub>S

**Molecular Weight:** 351.46 g/mol

**Smiles:** CCOC(=O)C1=CN=C(C=C1)C#CC2=CC3=C(C=C2)SCCC3(C)C

**Recommended concentration:** 1 μM



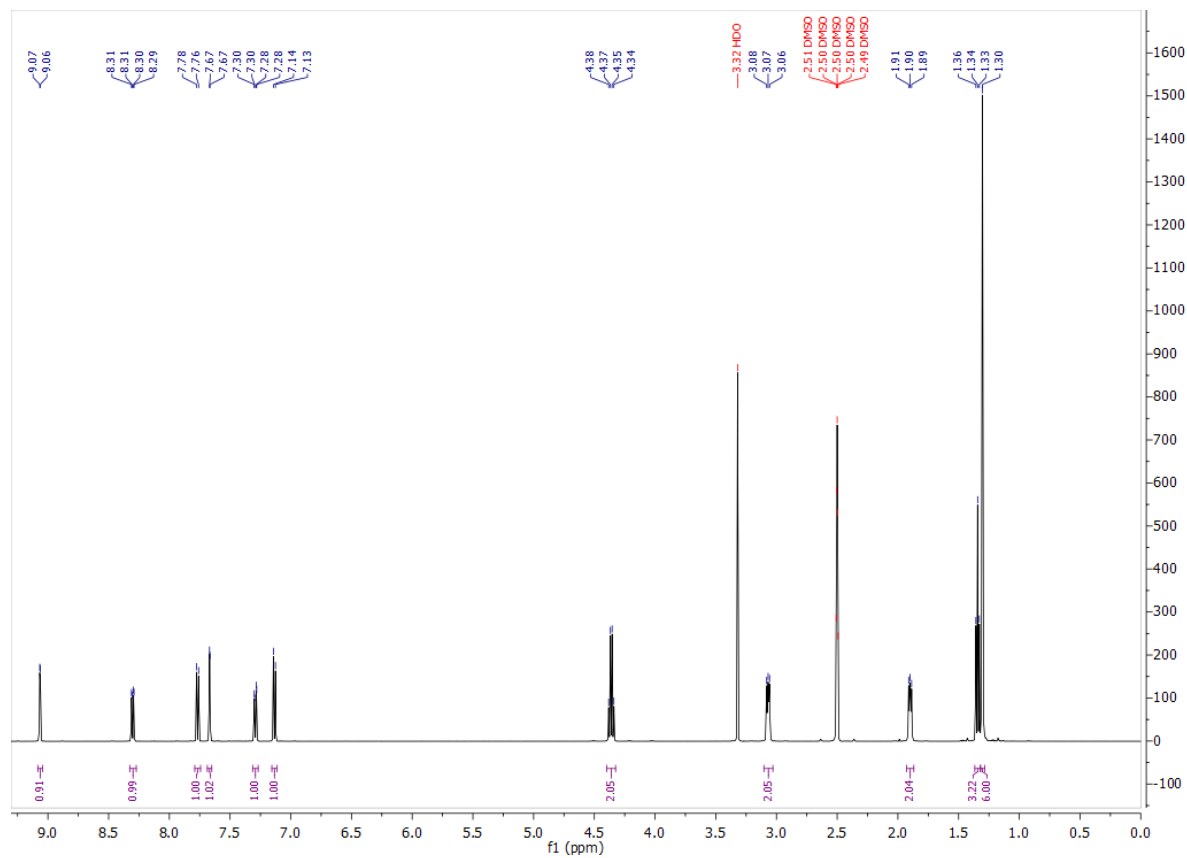
### Biological activity

	Type	IC <sub>50</sub> /EC <sub>50</sub> [μM]	Reference
Main NR target:	NR1B1 (RARα)	Agonist	0.06
	NR1B2 (RARβ)	Agonist	0.0008
	NR1B3 (RARγ)	Agonist	0.04
NR off-target:			<a href="https://doi.org/10.1016/j.bmcl.2008.11.040">https://doi.org/10.1016/j.bmcl.2008.11.040</a>

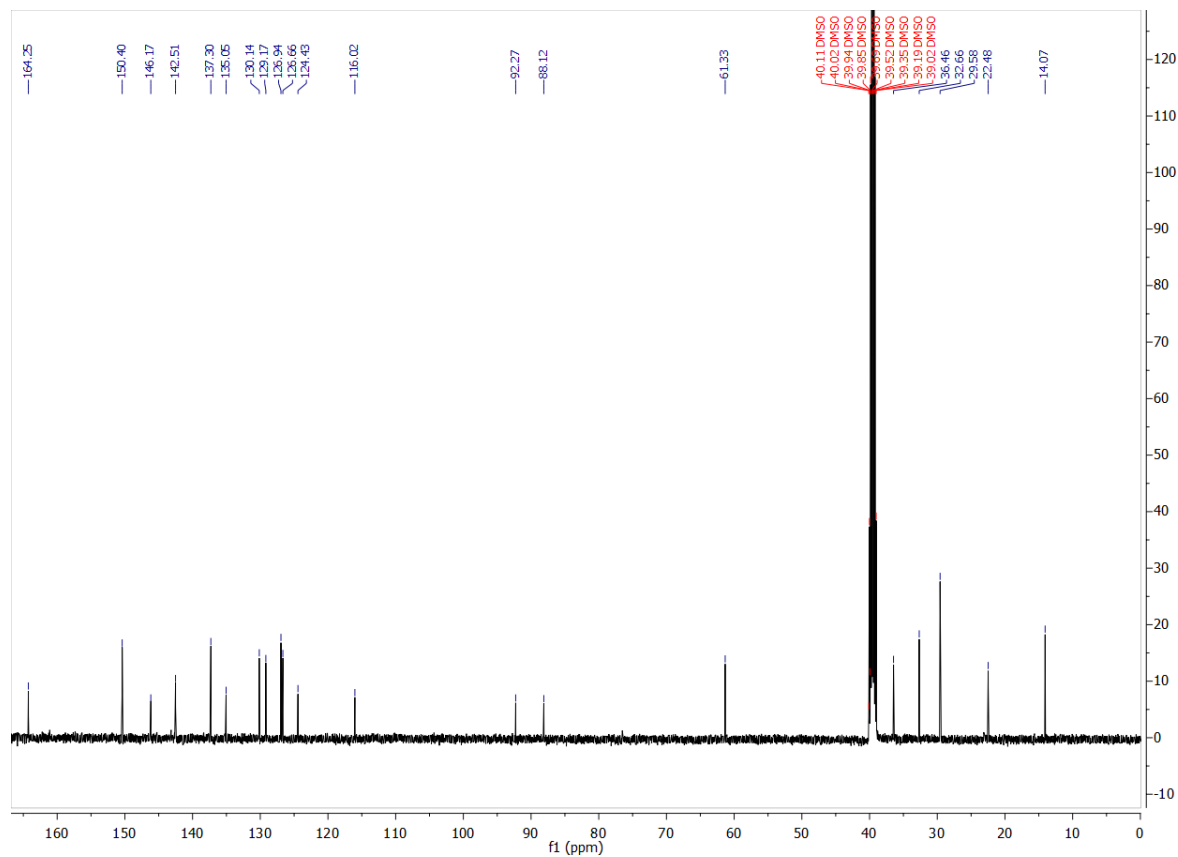
# COMPOUND INFORMATION

## Identity

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



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



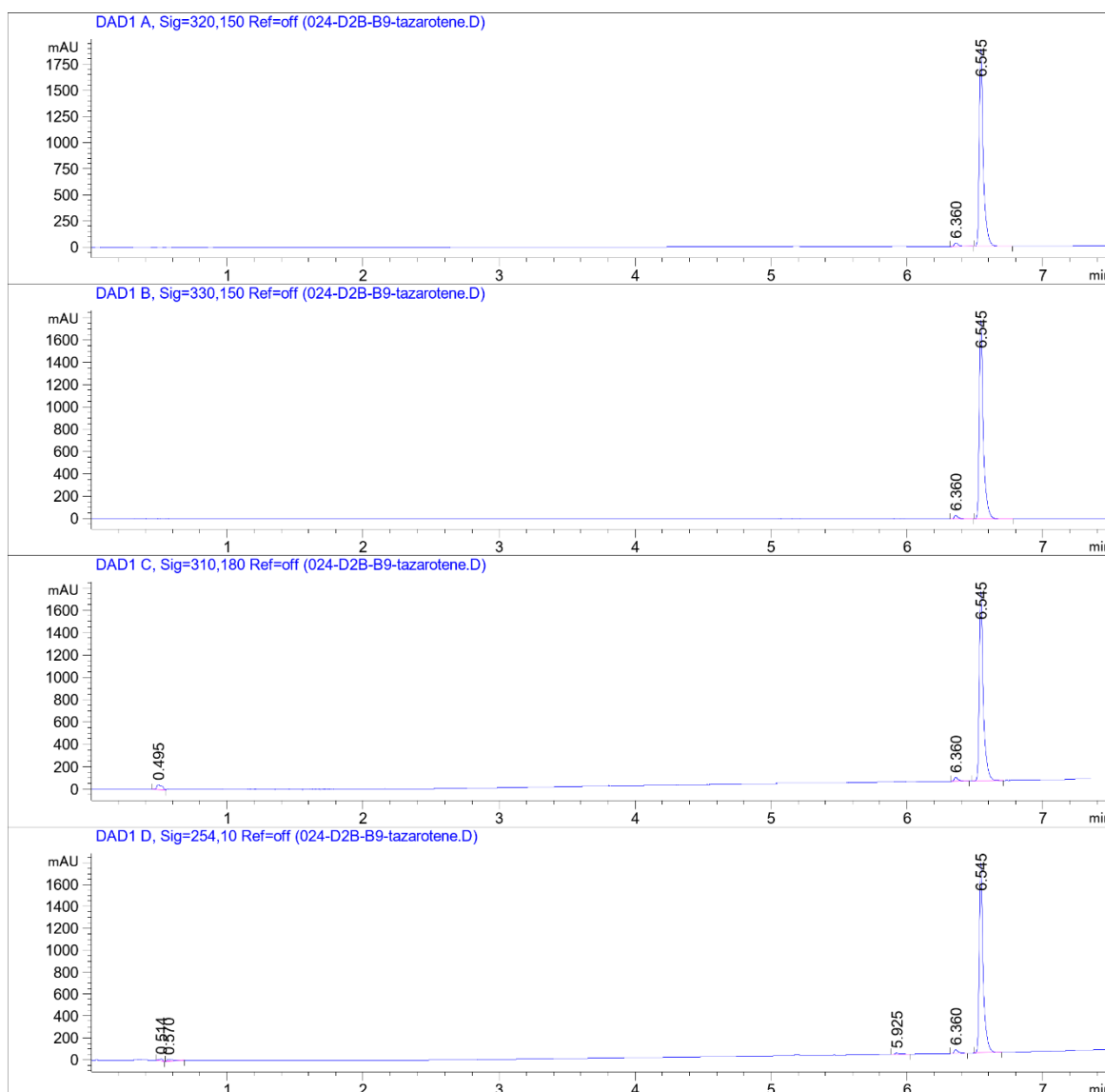
# COMPOUND INFORMATION

## Purity

Data File W:\analyti...\N\CGC\_ECH01-3\_FirstPass 2021-03-20 13-21-54\024-D2B-B9-tazarotene.D

Sample Name: tazarotene

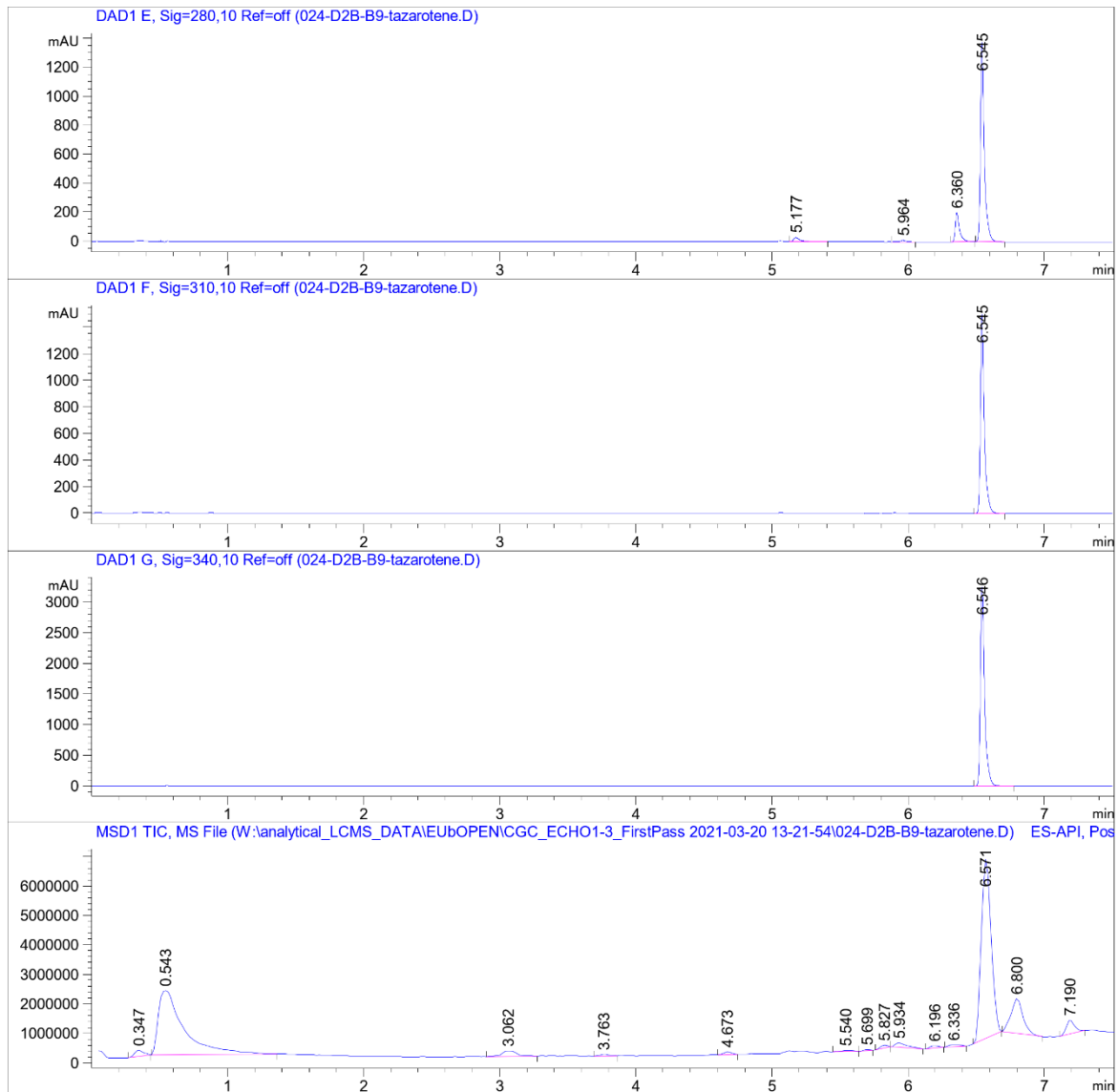
```
=====
Acq. Operator   : SYSTEM                      Seq. Line :   24
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2B-B9
Injection Date  : 3/20/2021 5:40:31 PM       Inj       :    1
                                           Inj Volume: Inj prog
Sequence File   : 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...\N\CGC\_ECH01-3\_FirstPass 2021-03-20 13-21-54\024-D2B-B9-tazarotene.D

Sample Name: tazarotene



# COMPOUND INFORMATION



Data File W:\analyti...\N\CGC\_ECH01-3\_FirstPass 2021-03-20 13-21-54\024-D2B-B9-tazarotene.D

Sample Name: tazarotene

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	937717	157.90 I
-	-	0.543	28776806	157.00 I
-	-	3.062	1403390	217.10 I
-	-	3.763	213235	274.20 I
-	-	4.673	390833	326.30 I
-	-	5.540	297630	326.30 I 295.20 I 282.30 I 280.20 I 102.10 I
-	-	5.699	152586	280.20 I
-	-	5.827	346908	296.20 I
-	-	5.934	843527	296.20 I 294.20 I 280.20 I
-	-	6.196	324168	280.20 I 228.20 I
6.360	71	6.336	379048	254.20 I
6.545	3847	6.571	30548758	352.10 I
-	-	6.800	7177743	282.20 I
-	-	7.190	1956745	284.20 I 282.20 I

