

## T3 (3,3',5-Triiodo-L-thyronine)

**CAS Registry No.:** 6893-02-3

**Formal Name:** (S)-2-amino-3-(4-(4-hydroxy-3-iodophenoxy)-3,5-diiodophenyl)propanoic acid

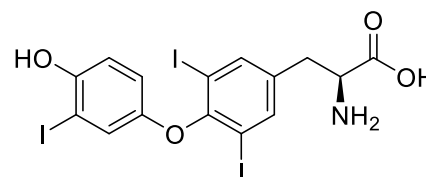
**EUBOPEN ID:** EUB0000555a

**Molecular Formula:** C<sub>15</sub>H<sub>12</sub>I<sub>3</sub>NO<sub>4</sub>

**Molecular Weight:** 650.98 g/mol

**Smiles:** C1=CC(=C(C=C1)OC2=C(C(=C(C=C2)I)I)O)N)I)O

**Recommended concentration:** 1 μM



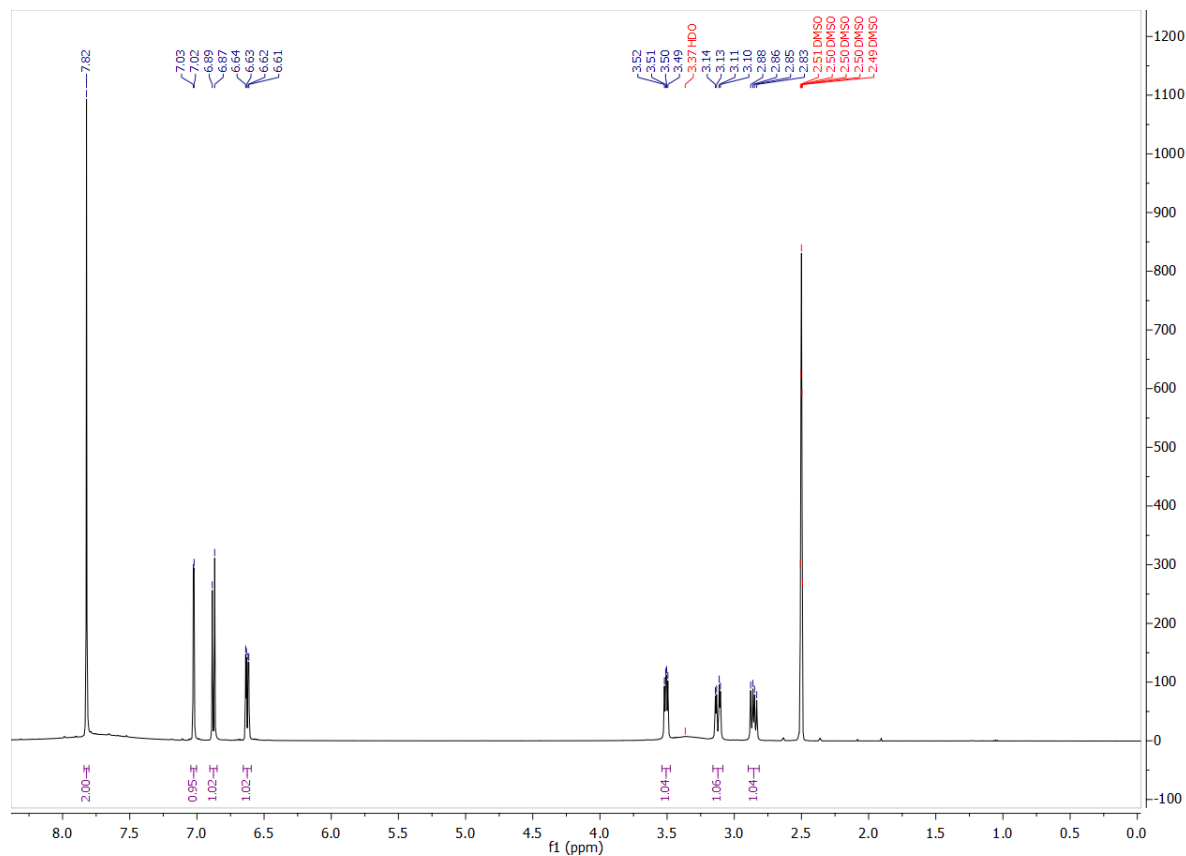
### Biological activity

		Type	IC <sub>50</sub> /EC <sub>50</sub> [μM]	Reference
Main NR target:	NR1A1 (THRα)	Agonist	0.002	<a href="https://doi.org/10.1016/j.bmc.2007.10.040">https://doi.org/10.1016/j.bmc.2007.10.040</a> , <a href="https://doi.org/10.1021/jm0201013">https://doi.org/10.1021/jm0201013</a>
	NR1A2 (THRβ)	Agonist	0.002	
NR off-target:				

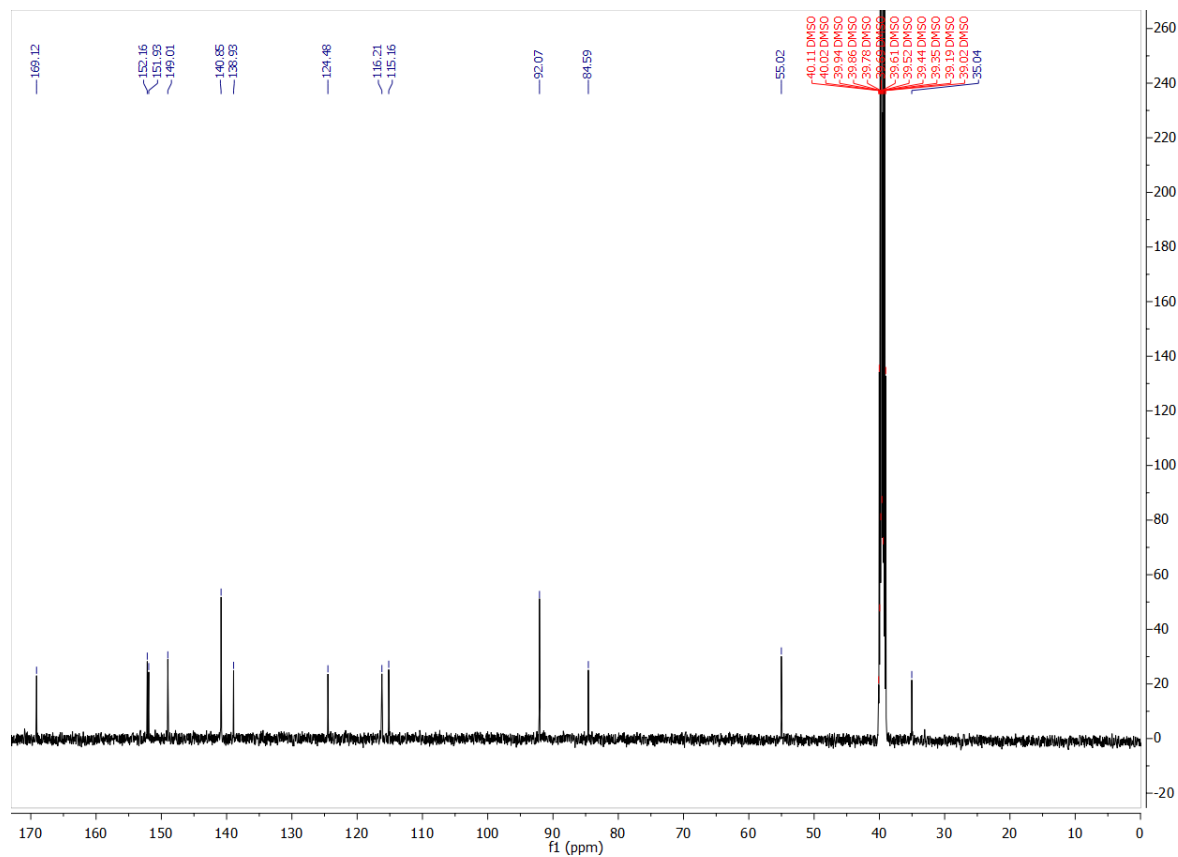
# COMPOUND INFORMATION

## Identity

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



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



# COMPOUND INFORMATION

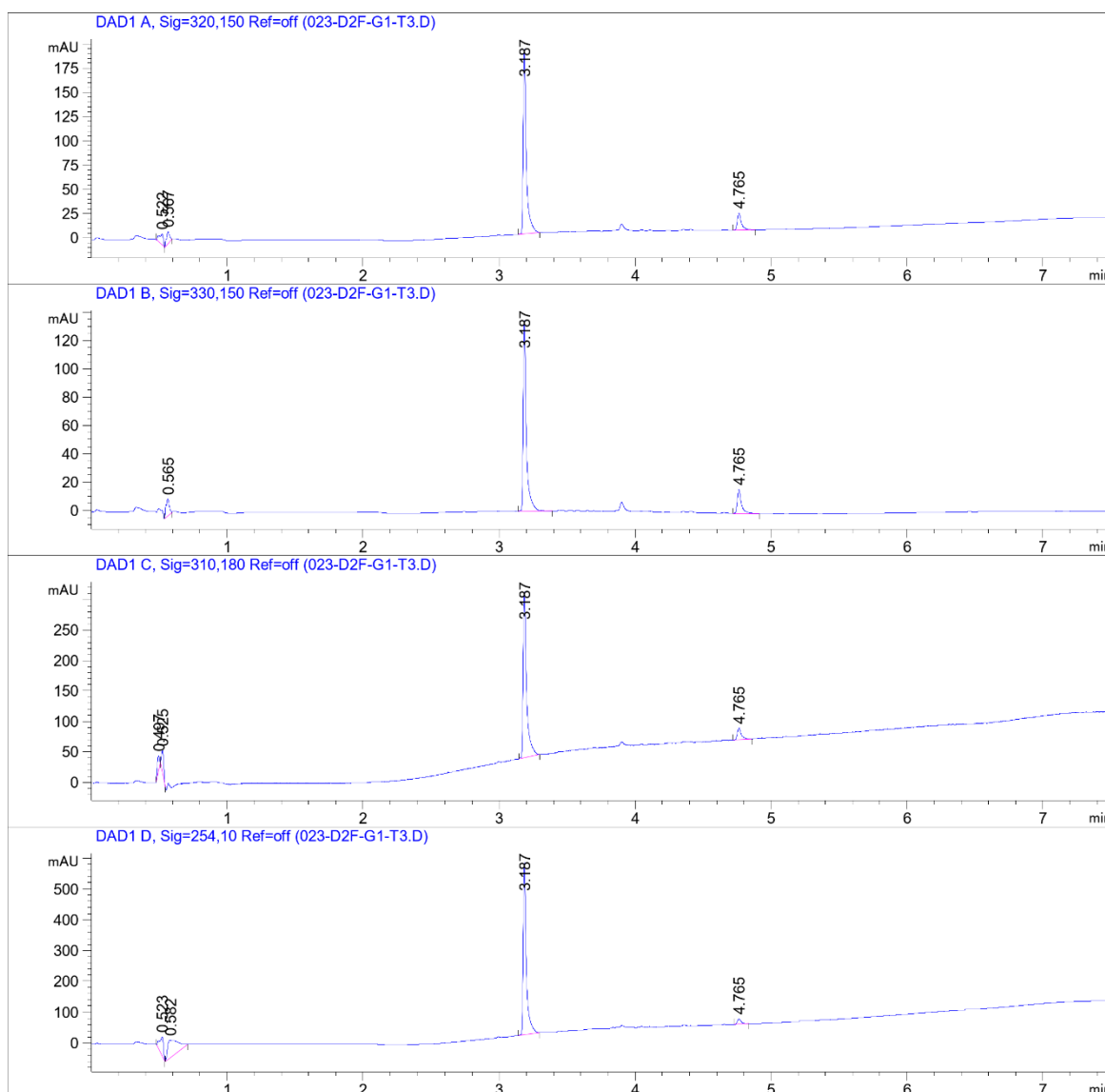
## Purity

Data File W:\analyti...\EubOPEN\CGC\_ECH01-2\_SecondPass 2021-03-23 18-53-53\023-D2F-G1-T3.D

Sample Name: T3

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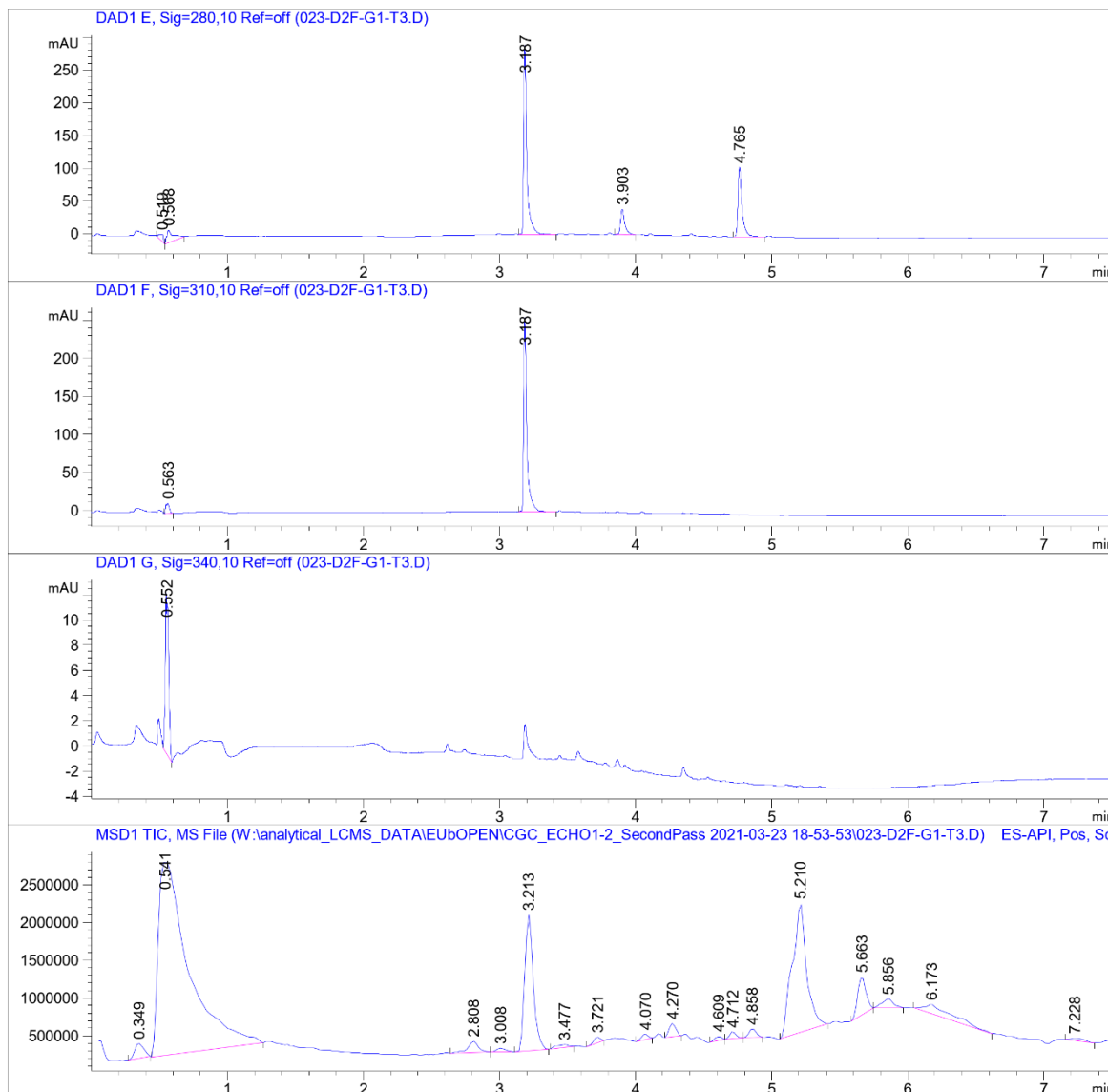
Acq. Operator	: SYSTEM	Seq. Line	: 23
Sample Operator	: SYSTEM		
Acq. Instrument	: LCMS test	Location	: D2F-G1
Injection Date	: 3/23/2021 11:01:33 PM	Inj	: 1
		Inj Volume	: Inj prog
Sequence File	: W:\analytical_LCMS_DATA\EubOPEN\CGC_ECH01-2_SecondPass 2021-03-23 18-53-53 CGC_ECH01-2_SecondPass.S		
Method	: W:\analytical_LCMS_DATA\EubOPEN\CGC_ECH01-2_SecondPass 2021-03-23 18-53-53 CGL_SECONDPASS_NONPOLCOMP_VIAL2+4_20210323.M (Sequence Method)		
Last changed	: 3/23/2021 6:50:05 PM by SYSTEM		
Method Info	: CGL wellplate, 0.5 uL of 10 mM DMSO. Dilution with MeCN only (9+9 uL)		



# COMPOUND INFORMATION

Data File W:\analyti...\EubOPEN\CGC\_ECH01-2\_SecondPass 2021-03-23 18-53-53\023-D2F-G1-T3.D

Sample Name: T3



# COMPOUND INFORMATION



Data File W:\analyti...\EubOPEN\CGC\_ECH01-2\_SecondPass 2021-03-23 18-53-53\023-D2F-G1-T3.D

Sample Name: T3

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	920387	200.00 I 183.10 I 159.00 I 142.00 I 111.10 I 110.10 I
0.522	23	0.541	39819696	157.10 I
0.567	20	-	-	
-	-	2.808	787438	217.10 I
-	-	3.008	213253	525.90 I 274.30 I 200.00 I 158.90 I 157.10 I
3.187	303	3.213	7789105	651.90 I
-	-	3.477	261675	232.10 I
-	-	3.721	263599	214.10 I
-	-	4.070	235858	216.10 I
-	-	4.270	594019	296.30 I
-	-	4.609	200004	280.30 I 228.20 I
4.765	37	4.712	282520	254.30 I
-	-	4.858	393240	280.30 I
-	-	5.210	12456643	282.30 I
-	-	5.663	2142663	359.30 I 341.30 I 284.30 I 282.20 I
-	-	5.856	623589	400.30 I 282.30 I
-	-	6.173	1855474	282.30 I
-	-	7.228	249470	102.20 I

