

Elafibranor

CAS Registry No.: 923978-27-2

Formal Name: (E)-2-(2,6-dimethyl-4-(3-(4-(methylthio)phenyl)-3-oxoprop-1-en-1-yl)phenoxy)-2-methylpropanoic acid

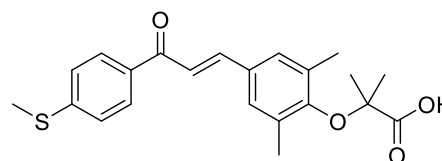
EUBOPEN ID: EUB0001147a

Molecular Formula: C₂₂H₂₄O₄S

Molecular Weight: 384.49 g/mol

Smiles: CC1=CC(=CC(=C1OC(C)(C)C(=O)O)C)C=CC(=O)C2=CC=C(C=C2)S

Recommended concentration: 1 μ M

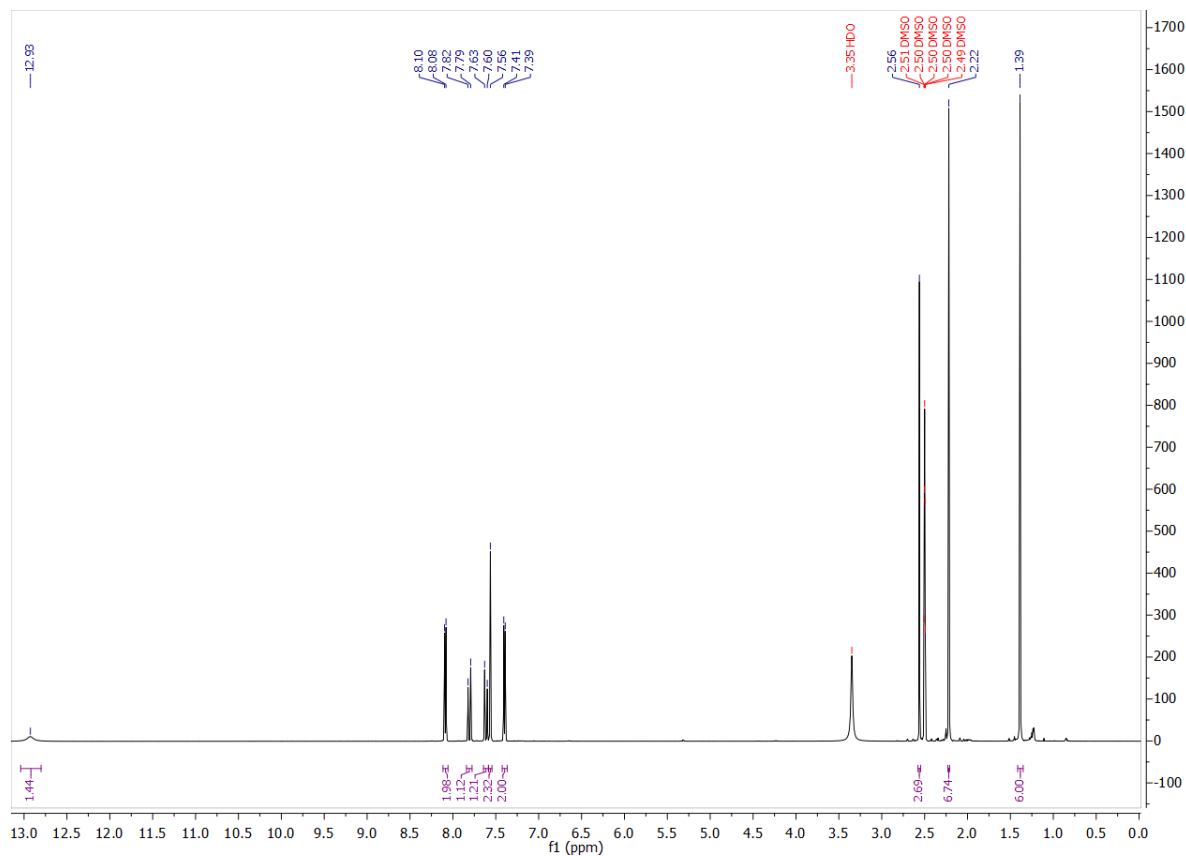


Biological activity

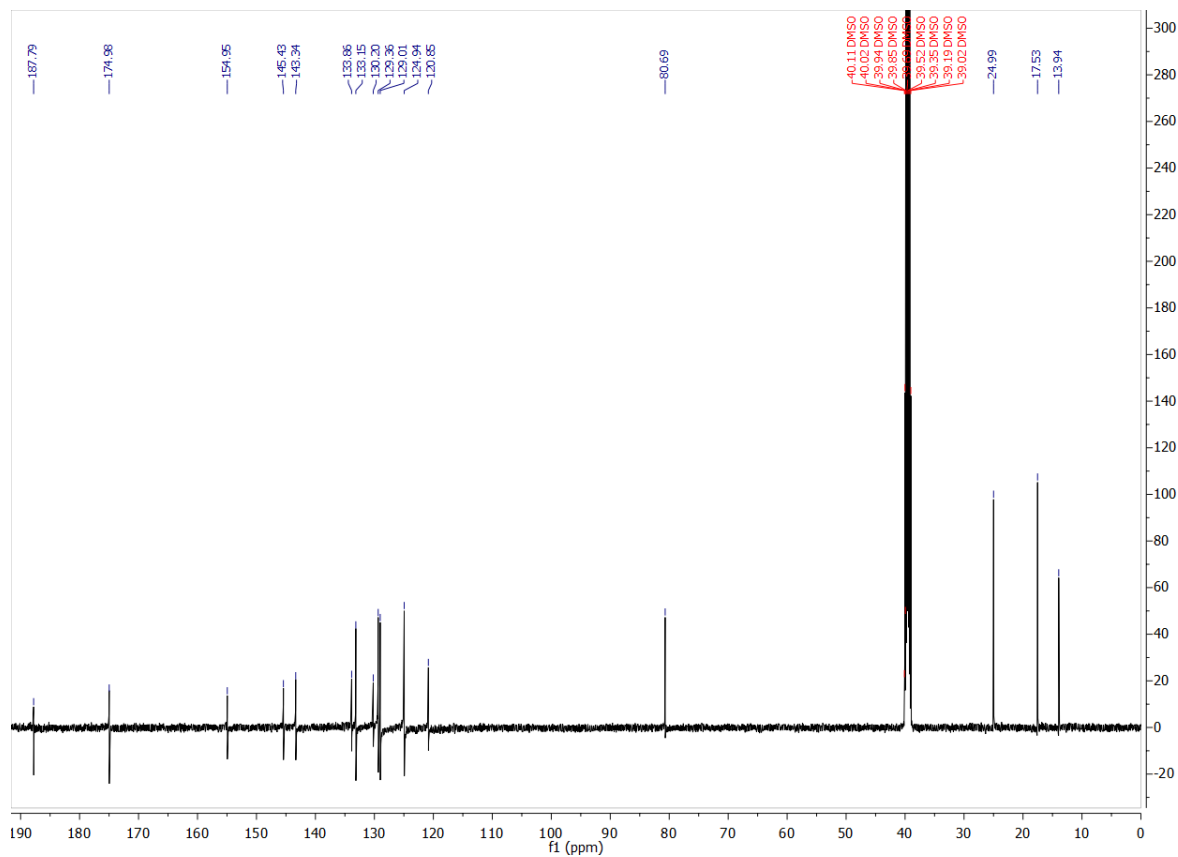
		Type	IC ₅₀ /EC ₅₀ [μ M]	Reference
Main NR target:	NR1C1 (PPAR α)	Agonist	0.13	inhouse
	NR1C2 (PPAR δ)	Agonist	0.21	
	NR1C3 (PPAR γ)	Agonist	0.41	
NR off-targets:				

Identity

¹H NMR



¹³C NMR



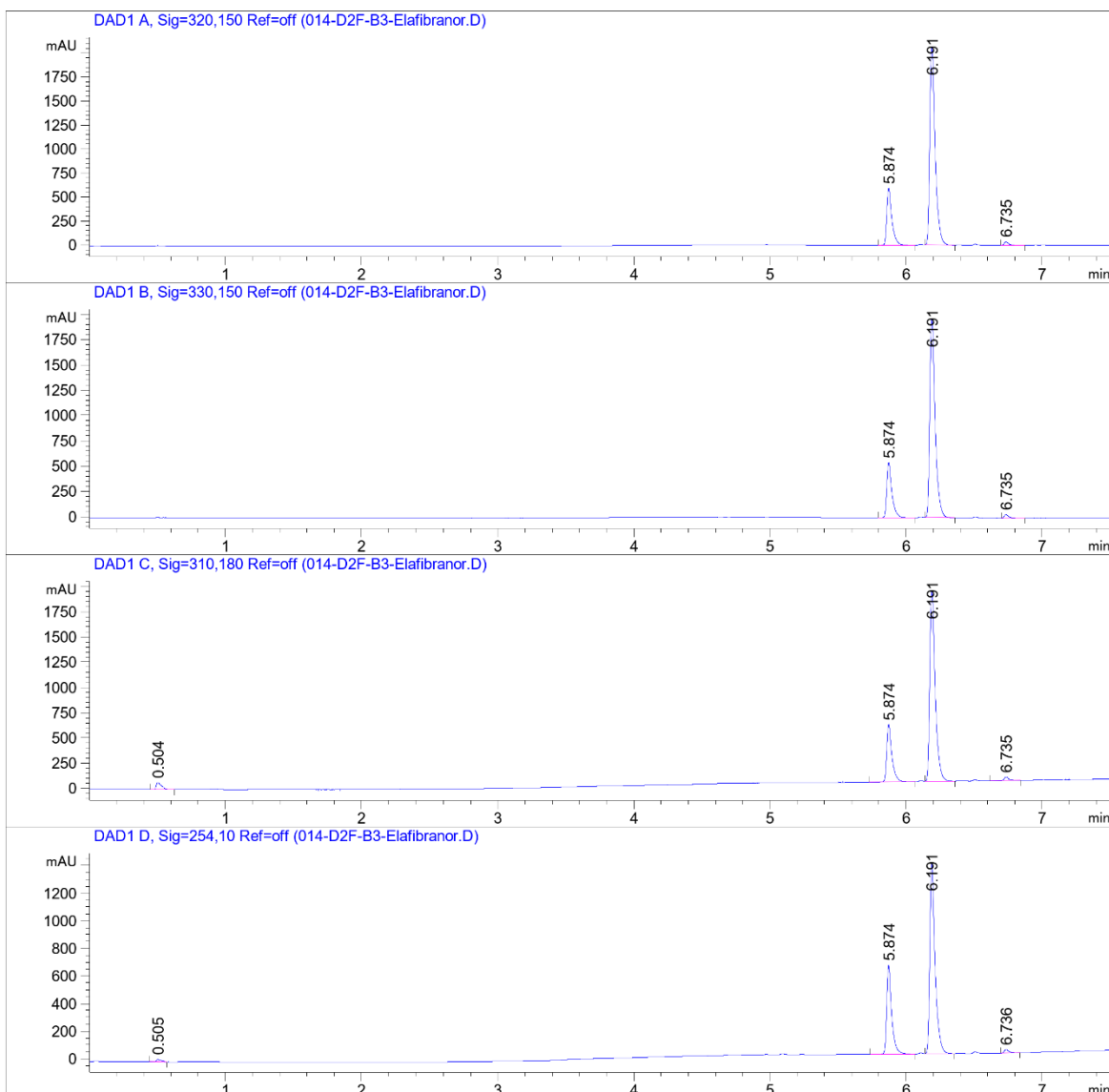
COMPOUND INFORMATION

Purity

Data File W:\analyti..._wave3_3rdRun_1stPassM 2023-05-05 17-35-57\014-D2F-B3-Elafibranor.D

Sample Name: Elafibranor

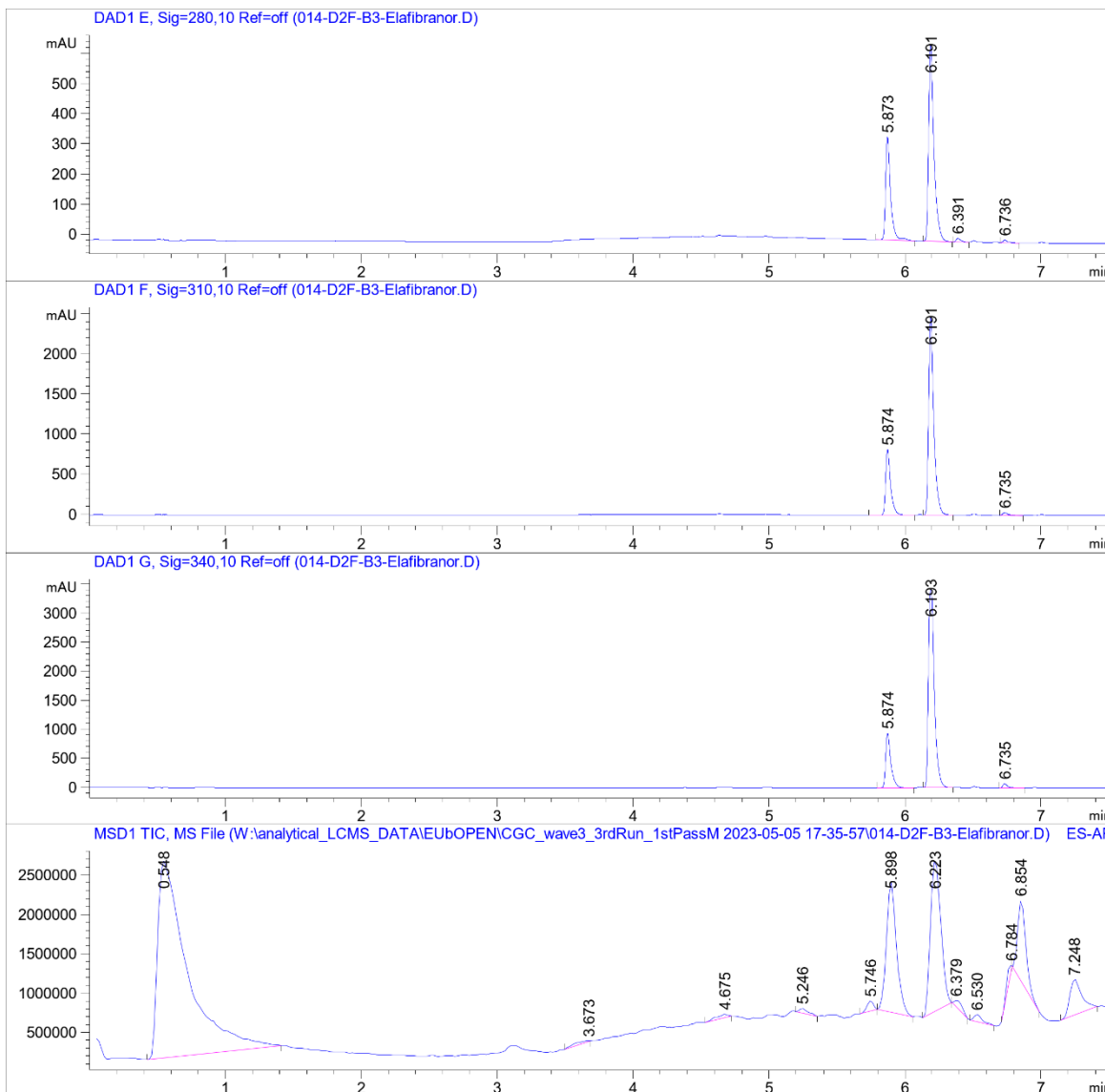
```
=====
Acq. Operator   : SYSTEM                      Seq. Line :   14
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2F-B3
Injection Date  : 5/5/2023 8:06:07 PM        Inj       :    1
                                           Inj Volume: Inj prog
Sequence File   : W:\analytical_LCMS_DATA\EUBOPEN\CGC_wave3_3rdRun_1stPassM 2023-05-05 17-35-
57\CGC_wave3_3rdRun_1stPassM.S
Method          : W:\analytical_LCMS_DATA\EUBOPEN\CGC_wave3_3rdRun_1stPassM 2023-05-05 17-35-
57\CGL_FIRSTPASS_GENERALMETHOD_VIAL1+2_20210319.M (Sequence Method)
Last changed    : 1/25/2022 4:36:18 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..._wave3_3rdRun_1stPassM 2023-05-05 17-35-57\014-D2F-B3-Elafibranor.D

Sample Name: Elafibranor



COMPOUND INFORMATION



Data File W:\analyti..._wave3_3rdRun_1stPassM 2023-05-05 17-35-57\014-D2F-B3-Elafibranor.D

Sample Name: Elafibranor

MS Signal: MSD1 TIC, MS File, ES-API, Pos, Scan, Frag: 70, "POS Scan"

Spectra from peak tops.

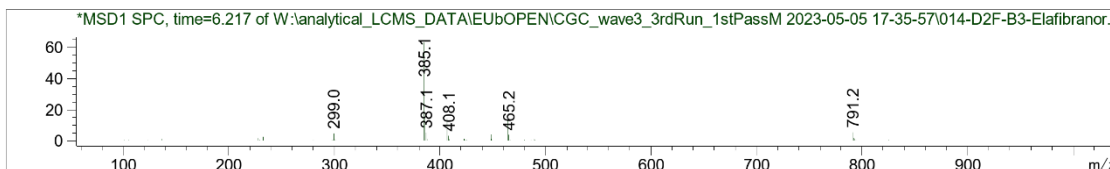
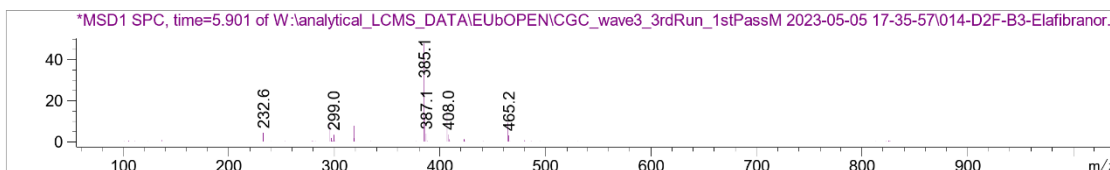
Noise Cutoff: 1000 counts.

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
-	-	0.548	38118588	157.00 I
-	-	3.673	236383	232.60 I
-	-	4.675	290988	232.70 I
-	-	5.246	273169	232.60 I
-	-	5.746	437644	280.20 I 232.60 I
5.874	1535	5.898	8512759	385.10 I
6.191	5651	6.223	10189516	385.10 I
-	-	6.379	362086	254.20 I 232.60 I 172.10 I
-	-	6.530	357444	341.10 I 280.20 I 232.70 I 137.10 I
6.735	87	6.784	415121	256.20 I
-	-	6.854	4355882	282.20 I
-	-	7.248	2698250	284.20 I



COMPOUND INFORMATION

Biological activity

