

MBX-8025 sodium salt (Seladelpar)

CAS Registry No.: 851528-79-5

Formal Name: Sodium (R)-2-(4-((2-ethoxy-3-(4-(trifluoromethyl)phenoxy)propyl)thio)-2-methylphenoxy)acetate

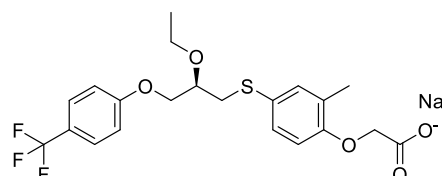
EUbOPEN ID: EUB0001145aNa

Molecular Formula: C₂₁H₂₂F₃NaO₅S

Molecular Weight: 466.45 g/mol

Smiles: CCOC(COC1=CC=C(C=C1)C(F)(F)F)CSC2=CC(=C(C=C2)OCC(=O)[O-])C.[Na+]

Recommended concentration: 1 μM



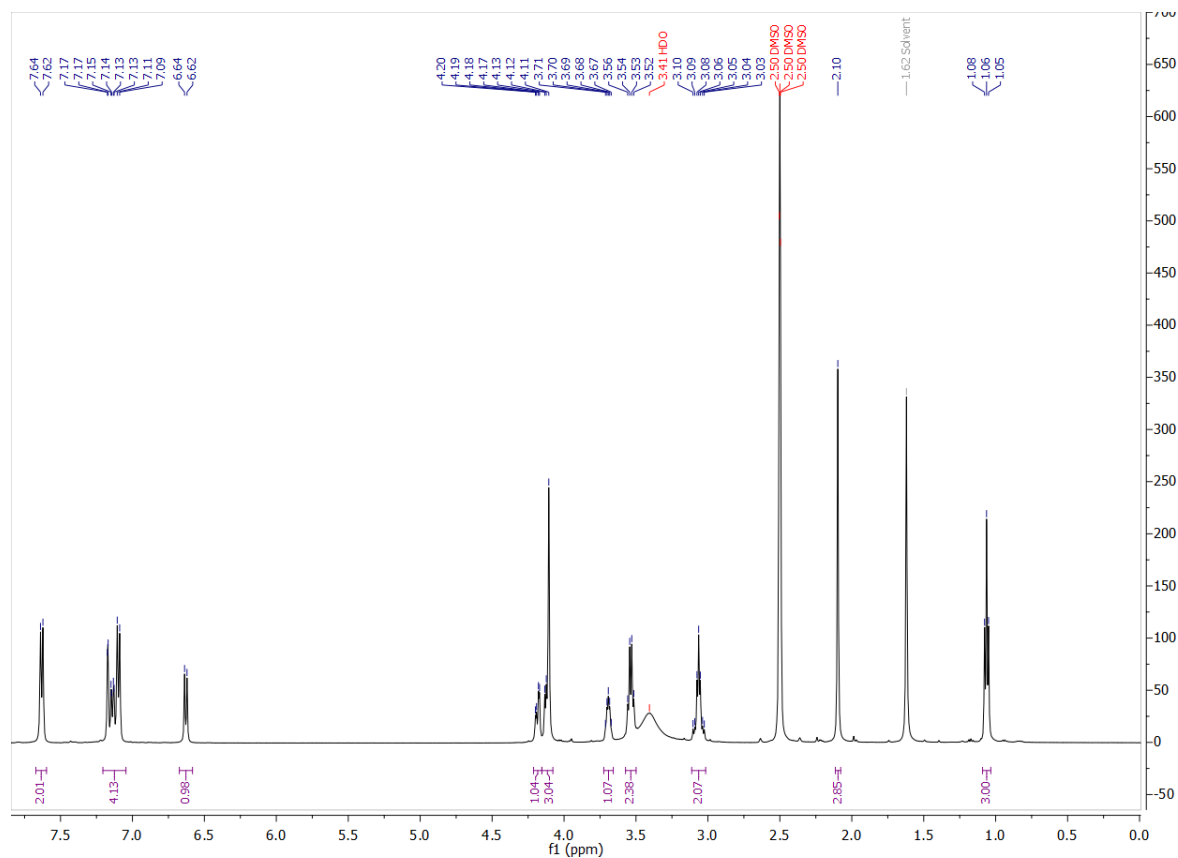
Biological activity

		Type	IC ₅₀ /EC ₅₀ [μM]	Reference
Main NR target:	NR1C2 (PPARδ)	Agonist	0.002	https://doi.org/10.1016/j.bmcl.2007.05.007
NR off-target:				

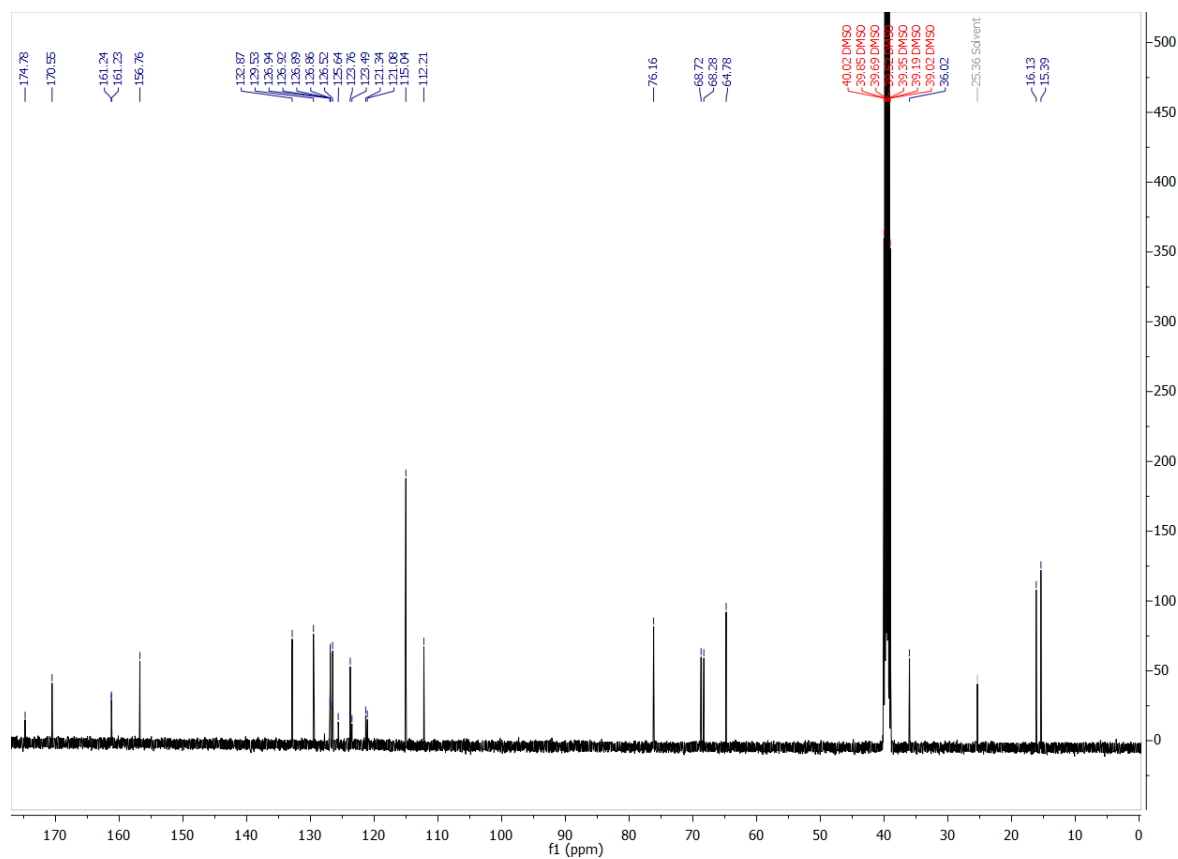
COMPOUND INFORMATION

Identity

¹H NMR



¹³C NMR



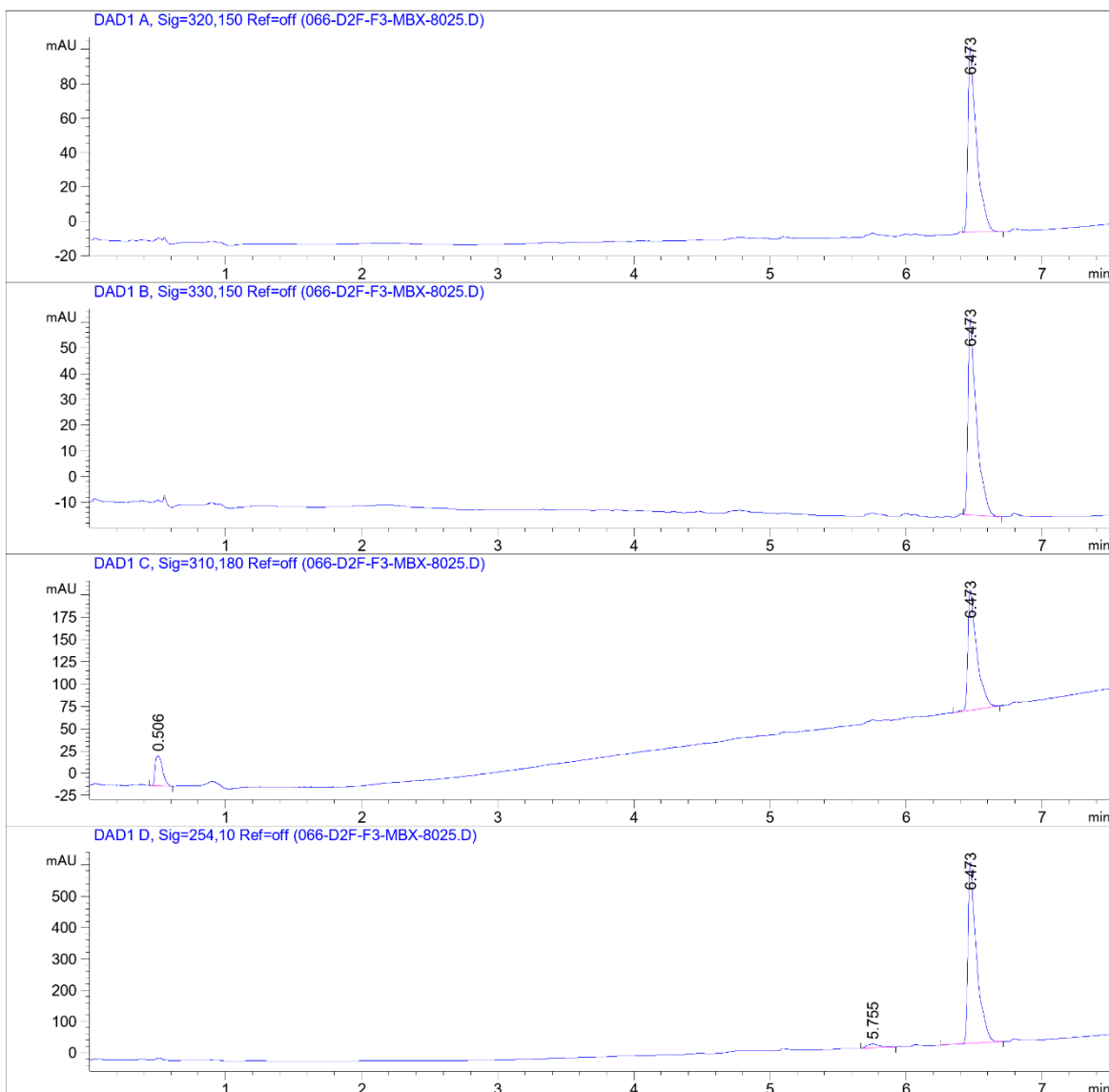
COMPOUND INFORMATION

Purity

Data File W:\analyti...EN\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\066-D2F-F3-MBX-8025.D

Sample Name: MBX-8025

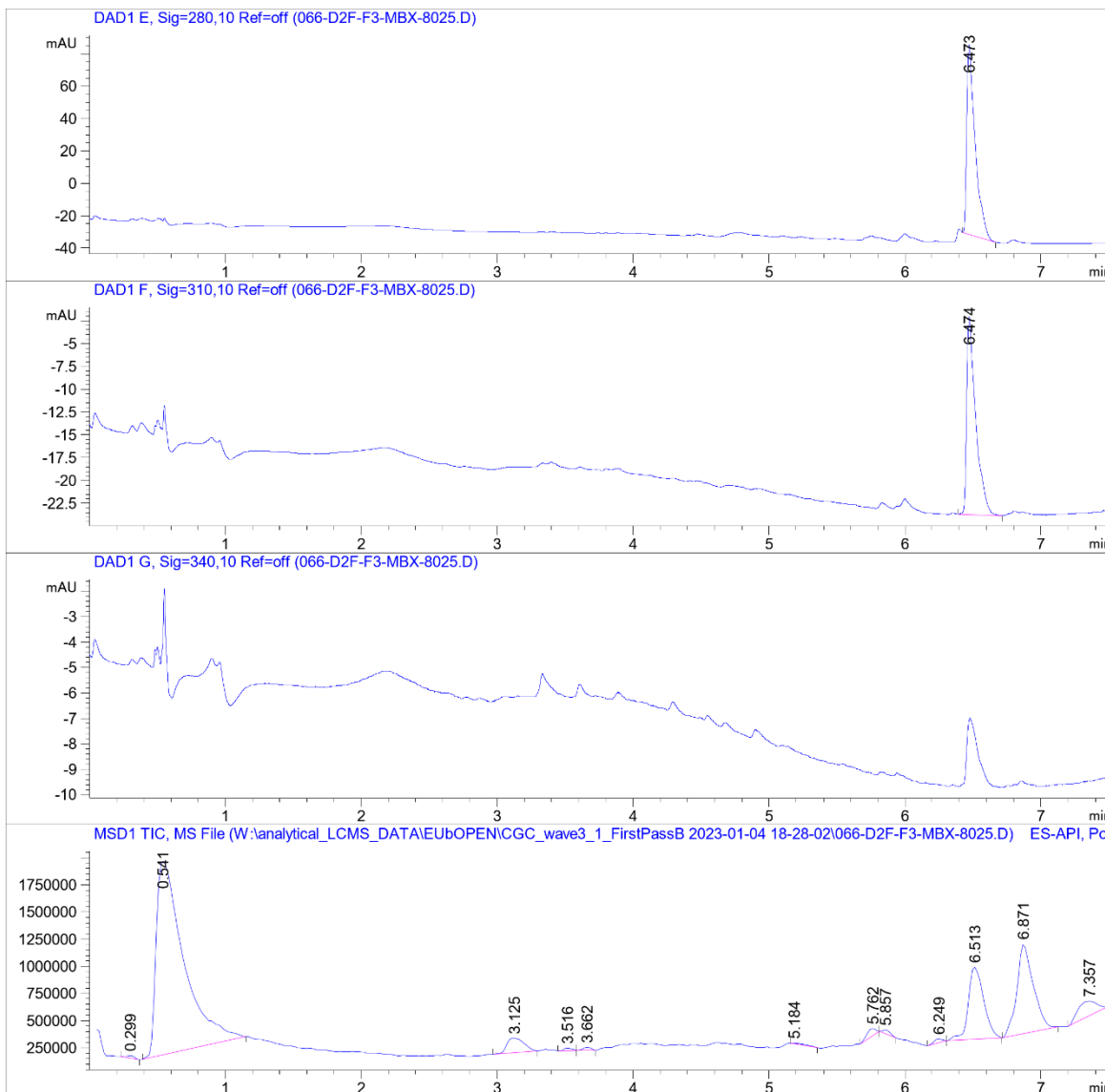
```
=====
Acq. Operator   : SYSTEM                      Seq. Line :   66
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2F-F3
Injection Date  : 1/5/2023 6:29:36 AM        Inj       :    1
                                           Inj Volume: Inj prog
Sequence File   : W:\analytical_LCMS_DATA\EUBOPEN\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02
                  \CGC_wave3_1_FirstPassB.S
Method          : W:\analytical_LCMS_DATA\EUBOPEN\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02
                  \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
=====
```



COMPOUND INFORMATION

Data File W:\analyti...EN\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\066-D2F-F3-MBX-8025.D

Sample Name: MBX-8025



COMPOUND INFORMATION

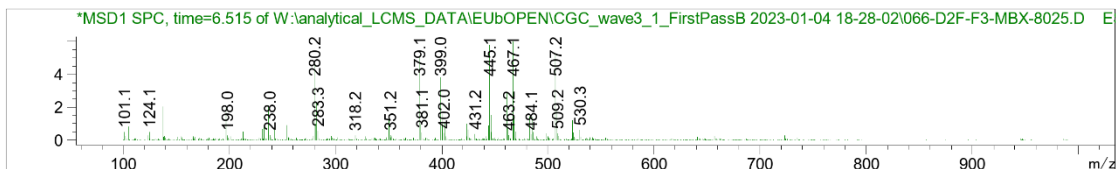


Data File W:\analyti...EN\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\066-D2F-F3-MBX-8025.D

Sample Name: MBX-8025

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
-	-	0.299	103602	200.00 I 159.00 I
-	-	0.541	25080690	157.10 I
-	-	3.125	1179300	239.10 I 217.10 I 188.10 I
-	-	3.516	103407	598.40 I 554.40 I 200.00 I 170.90 I 159.00 I
-	-	3.662	129922	170.80 I 158.90 I
-	-	5.184	87712	510.30 I 170.90 I 137.10 I
-	-	5.762	335804	461.10 I 280.30 I
-	-	5.857	146554	318.20 I 296.20 I
-	-	6.249	142514	228.20 I 137.10 I
6.473	472	6.513	5270303	507.20 I 467.10 I 445.10 I 399.00 I 379.10 I 280.20 I
-	-	6.871	6958635	282.20 I
-	-	7.357	1366345	400.30 I 282.30 I



COMPOUND INFORMATION

LC-MS

M_r 444.47

MS: ESI-negative, m/z 443/138 (blue), m/z 443/161 (red), m/z 443/385 (green)

LC: 0.1% HCOOH/ACN (30/70)

