

Bavachinin

CAS Registry No.: 19879-30-2

Formal Name: (S)-2-(4-hydroxyphenyl)-7-methoxy-6-(3-methylbut-2-en-1-yl)chroman-4-one

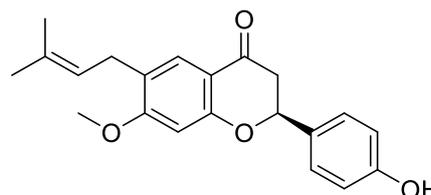
EUBOPEN ID: EUB0001143a

Molecular Formula: C₂₁H₂₂O₄

Molecular Weight: 338.40 g/mol

Smiles: CC(=CCC1=CC2=C(C=C1OC)OC(C2=O)C3=CC=C(C=C3)O)C

Recommended concentration: 1 μM

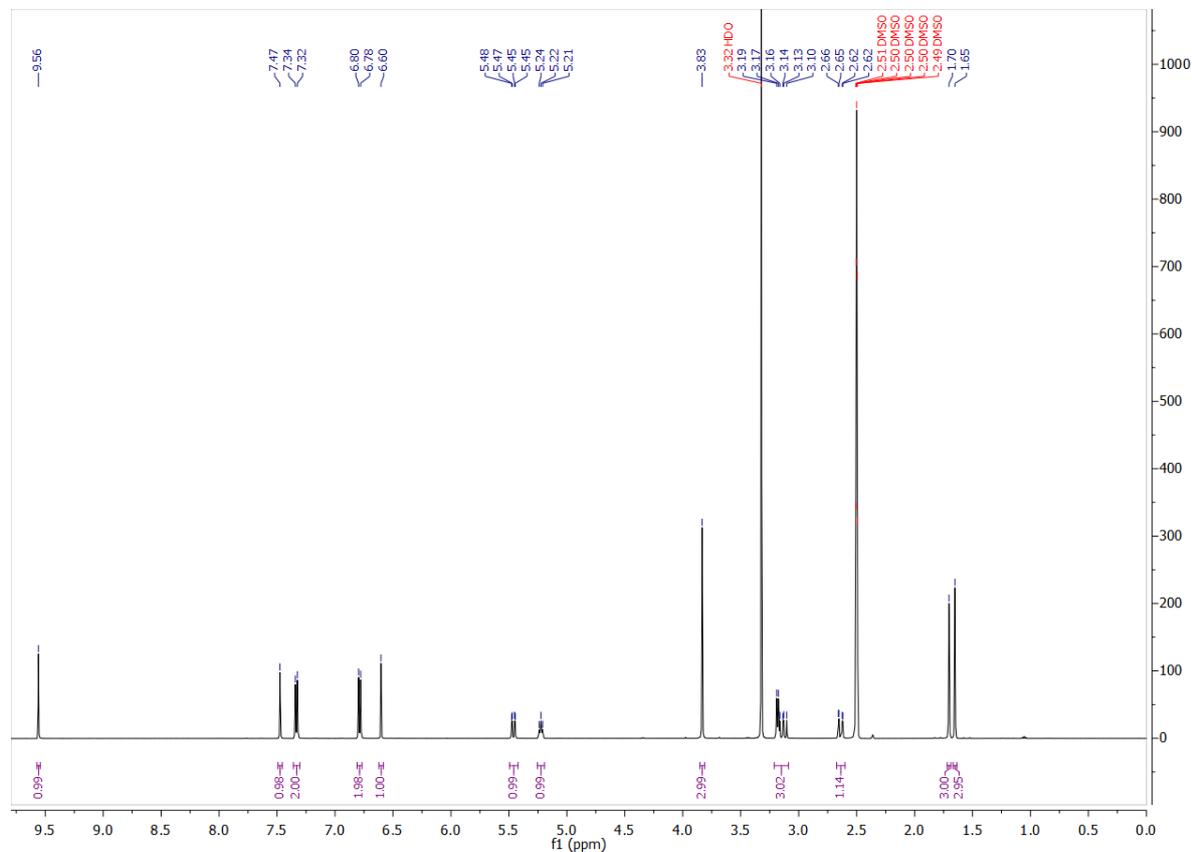


Biological activity

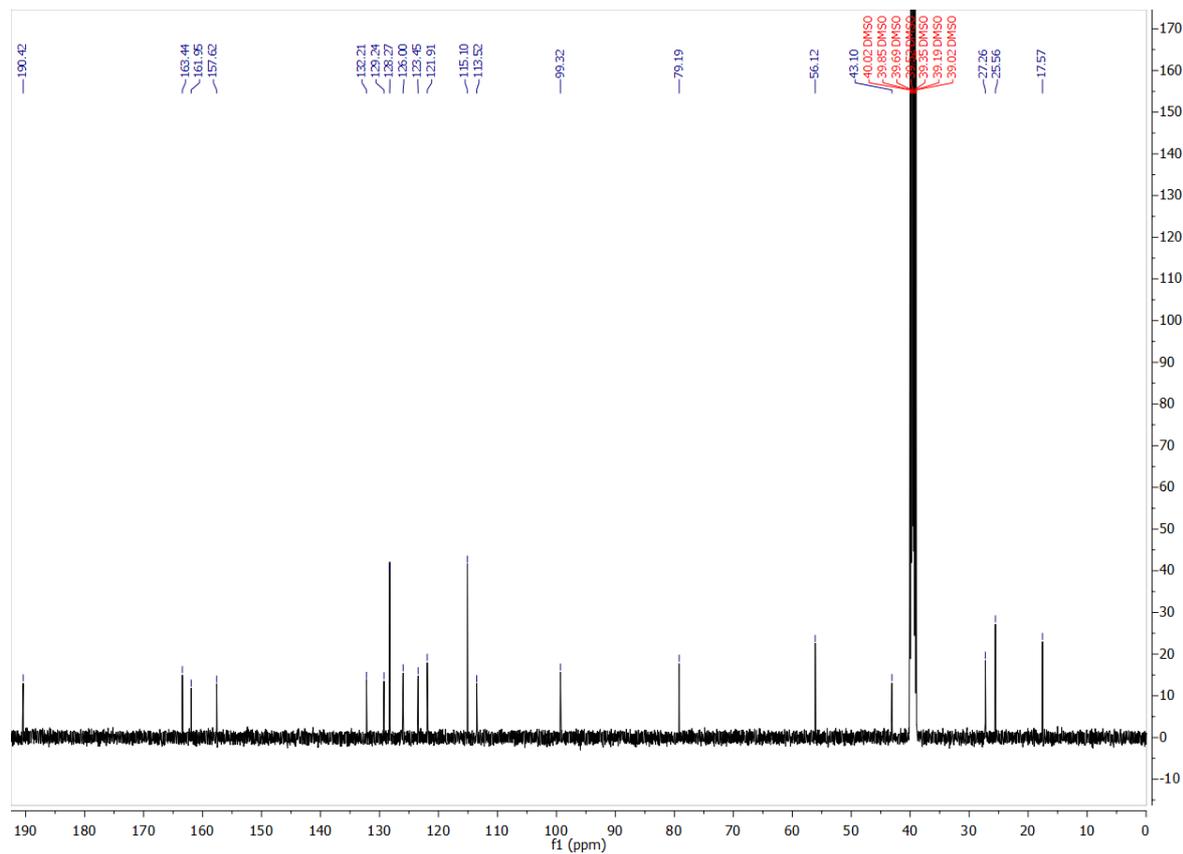
	Type	IC ₅₀ /EC ₅₀ [μM]	Reference
Main NR target:	NR1C3 (PPARγ) Agonist	0.7	https://doi.org/10.1007/s00125-016-3912-9
NR off-target:			

Identity

¹H NMR



¹³C NMR



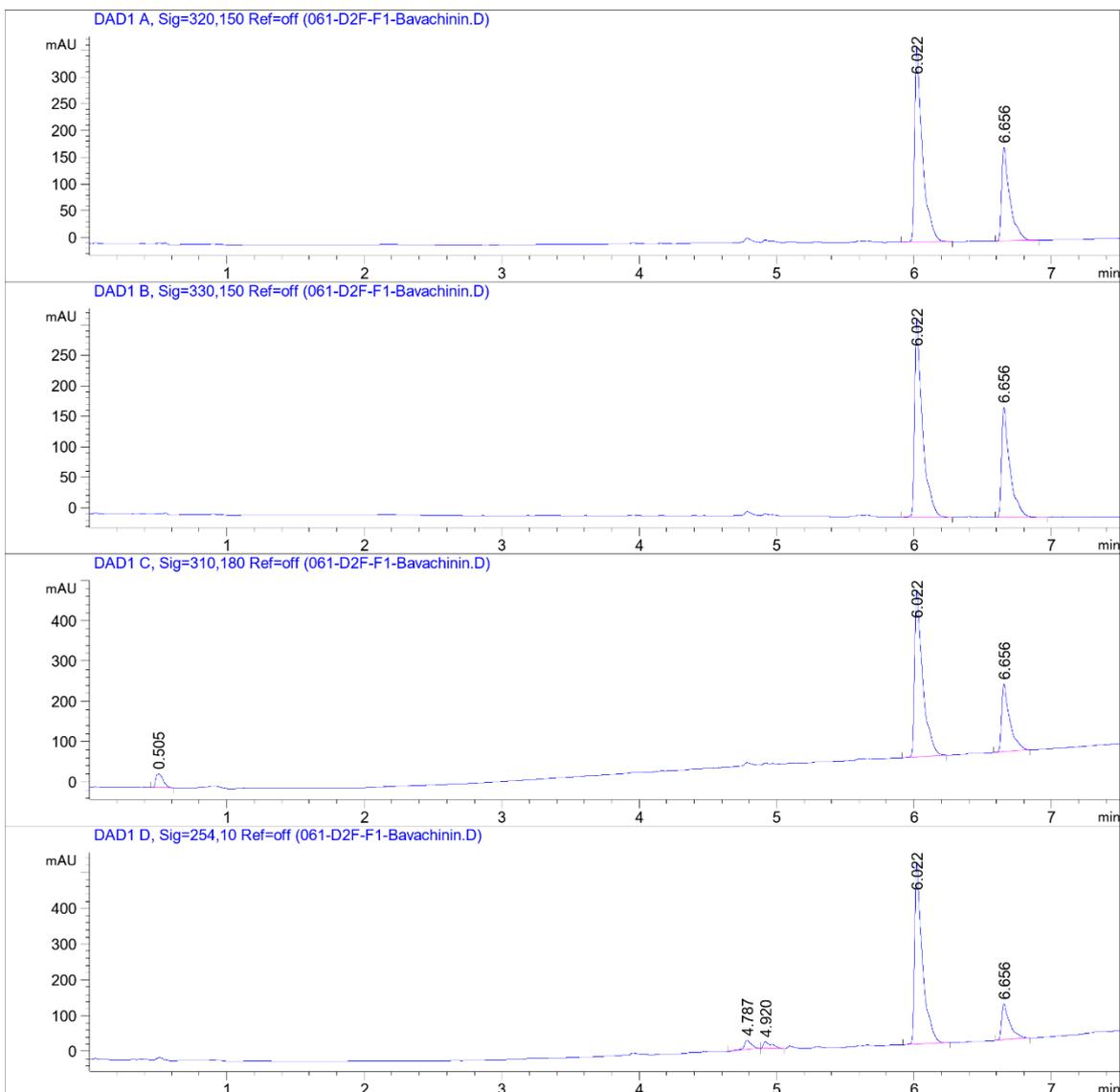
COMPOUND INFORMATION

Purity

Data File W:\analyti...\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\061-D2F-F1-Bavachinin.D

Sample Name: Bavachinin

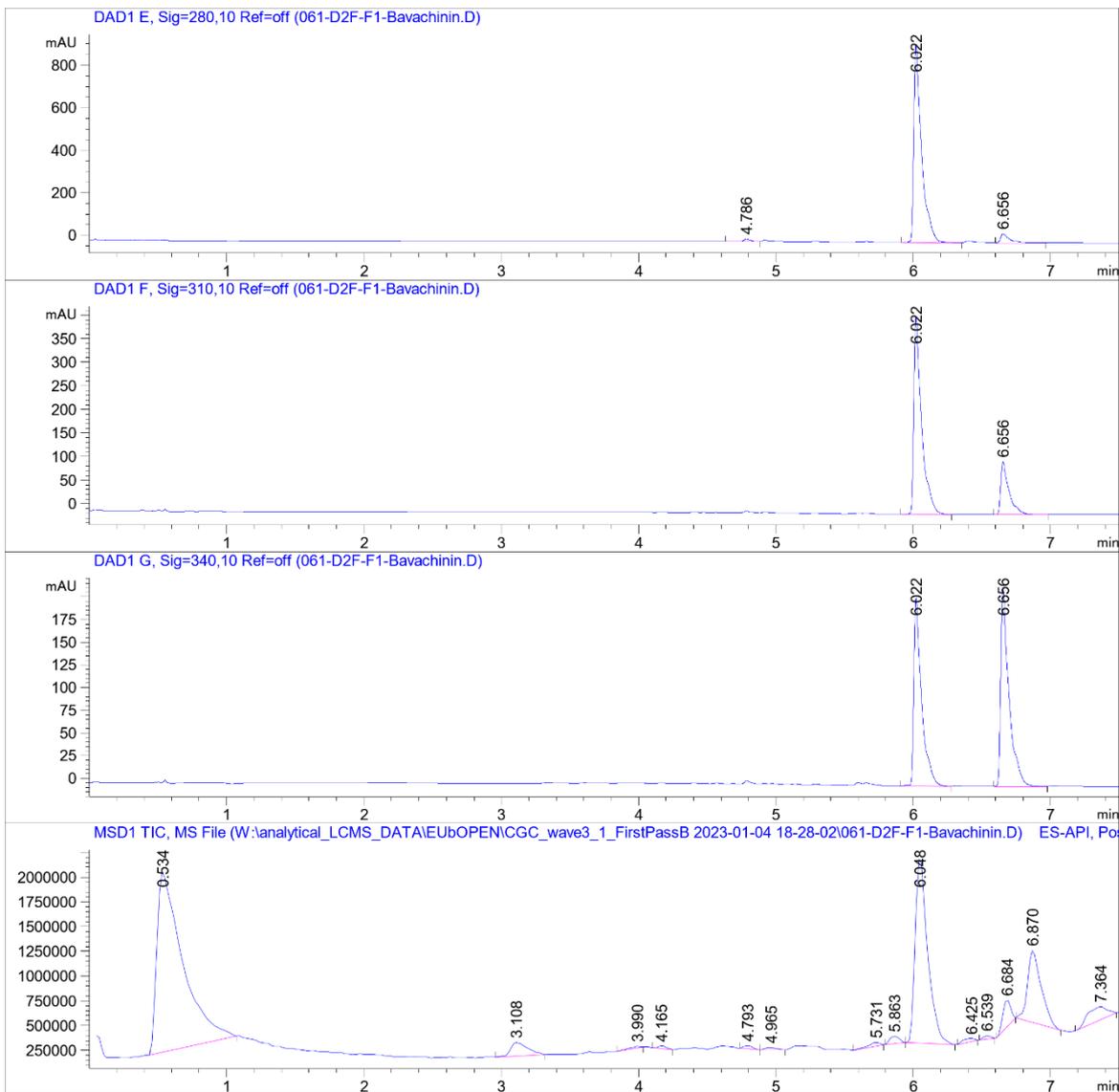
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=====
Acq. Operator   : SYSTEM                      Seq. Line :   61
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2F-F1
Injection Date  : 1/5/2023 5:34:18 AM         Inj       :    1
                                           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
=====
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COMPOUND INFORMATION

Data File W:\analyti...\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\061-D2F-F1-Bavachinin.D

Sample Name: Bavachinin



COMPOUND INFORMATION

Data File W:\analyti...\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\061-D2F-F1-Bavachinin.D

Sample Name: Bavachinin

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
-	-	0.534	23765002	157.00 I
-	-	3.108	1162701	239.10 I 217.10 I
-	-	3.990	116212	170.80 I
-	-	4.165	116257	170.80 I
-	-	4.793	145928	510.30 I 170.90 I
-	-	4.965	128429	510.30 I 170.90 I
-	-	5.731	224163	280.20 I
-	-	5.863	354805	318.20 I 296.20 I
6.022	1425	6.048	11734022	339.10 I
-	-	6.425	208327	350.20 I 282.20 I 254.20 I 137.10 I
-	-	6.539	132791	280.20 I
6.656	716	6.684	1056838	339.10 I
-	-	6.870	5085602	282.20 I
-	-	7.364	1380681	400.30 I 282.30 I

